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Solutions of the Klein-Gordon equation in an infinite square-well potential with a moving wall

M. Koehn

Max-Planck-Institut für Gravitationsphysik, Albert-Einstein-Institut - Am Mühlenberg 1, 14476 Potsdam, Germany, EU

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Abstract – Employing a transformation to hyperbolic space, we derive in a simple way exact solutions for the Klein-Gordon equation in an infinite square-well potential with one boundary moving at constant velocity, for the massless as well as for the massive case.

Introduction. – The *non-relativistic* system of a one-dimensional infinite square well including a massive particle evolving according to the Schrödinger equation is one of the most elementary quantum-mechanical systems, often serving as an approximation to more complex physical systems. If the potential walls are however not static but moving, as originally in the Fermi-Ulam model for the acceleration of cosmic rays [1,2], the situation is much more complicated: if one does not choose to rely on an adiabatic approximation, then the system is not separable anymore. Results concerning exact solutions exist only sparsely and have attracted a considerable amount of attention. For the special case of a non-relativistic system with a wall moving at constant velocity, such exact solutions have been obtained first in [3], see [4–6] for generalizations.

The *relativistic* moving-wall system is however a much less common object of study, and there appear interesting subtleties. We investigate the one-dimensional Klein-Gordon (KG) particle in an infinite square well with one static boundary and one boundary which is moving outward at constant velocity ν, and we find an infinite set of exact solutions which do not rely on an adiabatic approximation on top of the square-well approximation with definite position and momentum configuration. We thereby generalize the solutions presented in the appendix of [7], which are valid only for a special case and which are stated without specifying any method on how to obtain them. In contrast, we use a transformation to hyperbolic space which provides in a simple and new manner a set of general solutions for the massless as well as for the massive case, while introducing derivatives of first order into the transformed KG equation.

Exact solution. – The system we investigate is described as the initial/boundary value problem

$$\begin{cases} \dfrac{\partial^2}{\partial t^2}\Psi(t,x)=\dfrac{\partial^2}{\partial x^2}\Psi(t,x)-m^2\Psi(t,x), & \text{in } \mathcal{F}, \\ \Psi|_{\partial\mathcal{F}}=0, & \text{on } \partial\mathcal{F}, \\ \Psi(t_0,x)=f(x), \qquad (\partial_t\Psi)(t_0,x)=g(x) \end{cases} \tag{1}$$

with the infinite square well specified by the domain $\mathcal{F}=[0,L(t)]$ in terms of the length function $L(t)=L_0+\nu(t-t_0)$, where ν denotes the speed of the receding wall, $0<\nu<1$, $\partial\mathcal{F}$ denotes the boundary of $\mathcal{F}$, and $t,x\in\mathbb{R}$. We have rescaled the speed of light and Planck's constant to $c=1=\hbar$, and we will treat the massless case $m=0$ first. Although indeed leading to motionless walls, the transformation

$$x\mapsto x'=\frac{x}{L(t)} \tag{2}$$

which is usually applied in such a scenario (see, *e.g.*, [4,5] for the non-relativistic case) is of not much help in obtaining analytic solutions for the relativistic moving-wall system since unlike the Schrödinger equation, the KG equation is of second order in time.

However, by slicing the forward lightcone in $(1+1)$-dimensional Minkowski space in terms of hyperboloids and transforming to hyperbolic coordinates (cf. fig. 1), we obtain an infinite square-well system with static boundaries and with the hyperbolic radial coordinate ρ as the new time-like coordinate. Explicitly, the transformation is given by

$$t=\rho\gamma_t, \qquad x=\rho\gamma_x, \tag{3}$$

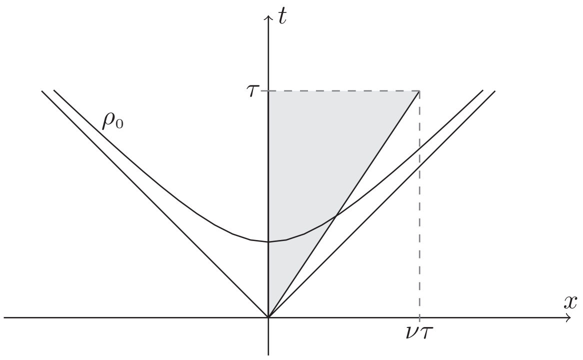


Fig. 1: Sketch of the infinite square well with moving walls as a shaded wedge inside the forward lightcone. It is depicted schematically how the wedge is intersected by a spacelike hyperboloid of fixed $\rho = \rho_0$.

subject to the constraint

$$(\gamma_t)^2 - (\gamma_x)^2 = 1 \tag{4}$$

which implies that $\rho^2 = t^2 - x^2$.

Since the γ coordinates are constrained to lie on the hyperboloid, one of the two coordinates is redundant. We parametrize by using coordinates on the one-dimensional analogue of the hyperbolic upper half-plane through

$$\gamma_t = \frac{v^2+1}{2v}, \qquad \gamma_x = \frac{v^2-1}{2v}, \qquad v = \gamma_t + \gamma_x. \tag{5}$$

In the hyperbolic coordinates, we are able to find a full set of exact solutions if we require as an intermediate step that $L_0 = \nu t_0$. We may afterwards freely shift the tip of the lightcone in order to obtain solutions for general parameters (L_0, t_0). After the transformation to hyperbolic space, the time dependence of the right boundary drops out and its position depends merely on the constant velocity. Employing (5), we can determine the position of the right boundary in hyperbolic space as (cf. fig. 2)

$$\Lambda(\nu) = \sqrt{\frac{1+\nu}{1-\nu}}, \tag{6}$$

while the transformed massless KG equation reads

$$\rho\partial_\rho\left(\rho\partial_\rho\Psi(\rho,v)\right) = v\partial_v\left(v\partial_v\Psi(\rho,v)\right). \tag{7}$$

Due to the separability of the system in hyperbolic coordinates, the general solution is given by

$$\Psi(\rho,v) = \psi_1(\rho v) + \psi_2(\rho/v), \tag{8}$$

where $\rho v = t + x$ and $\rho/v = t - x$, and we can easily choose a solution that matches the Dirichlet boundary conditions, *e.g.*,

$$\Psi_n(\rho,v) = \frac{1}{\sqrt{n\pi}}\sin\left(k_n \ln(v)\right)\exp(-\mathrm{i}k_n\ln(\rho)) \tag{9}$$

with

$$k_n = \frac{n\pi}{\ln(\Lambda(\nu))}. \tag{10}$$

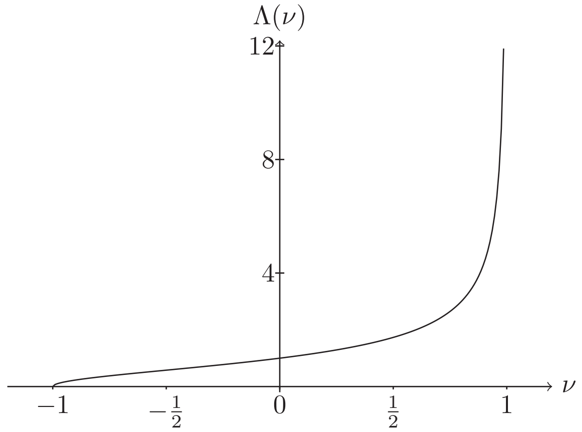


Fig. 2: Plot of the function Λ depending on the speed ν of the moving wall

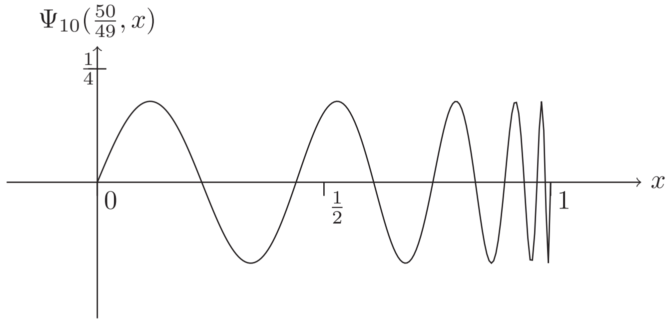


Fig. 3: Plot of the function $\Psi_{10}(\frac{50}{49}, x)$ with the speed $\nu = \frac{49}{50}$ of the moving wall.

The massive case corresponding to $\partial_t^2\Phi = \partial_x^2\Phi - m^2\Phi$ can be treated similarly, leading to the solutions

$$\Phi_n(\rho,v) = C\sin\left(k_n\ln(v)\right)\left[J_{\mathrm{i}k}(m\rho) + Y_{\mathrm{i}k}(m\rho)\right], \tag{11}$$

where $J_{\mathrm{i}k}$ and $Y_{\mathrm{i}k}$ are Bessel functions of imaginary order $\mathrm{i}k$. Of course we could have also chosen real solutions to the real KG equation. We remark that in a general number of dimensions, having a definite direction of wave packet propagation is related to complexity of the wave function.

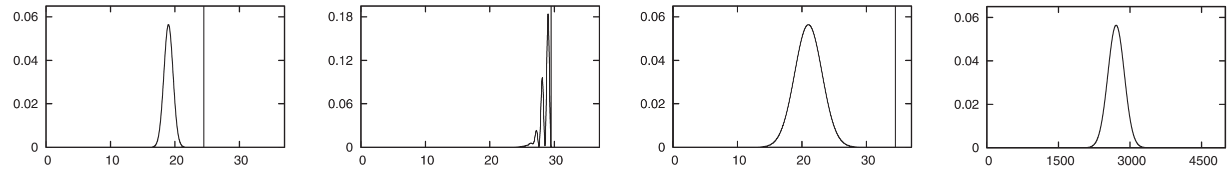
The solutions (9) are normalized to 1 with respect to the KG-like scalar product

$$(\psi_1,\psi_2) = \mathrm{i}\rho\int \mathrm{dvol}\,\psi_1^*\overleftrightarrow{\partial_\rho}\psi_2, \tag{12}$$

where $\psi\overleftrightarrow{\partial_\rho}\phi \equiv \psi\partial_\rho\phi - \phi\partial_\rho\psi$ and where $\mathrm{dvol} = \frac{\mathrm{d}v}{v}$ denotes the volume element on the one-dimensional hyperbolic upper half-plane. We can express the solutions (9) in flat coordinates as

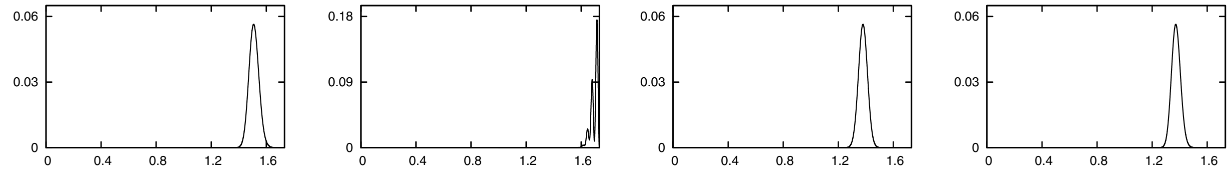
$$\begin{aligned}\Psi_n(t,x) \;=\; & \frac{1}{\sqrt{n\pi}}\sin\left[\frac{k_n}{2}\ln\left(\tfrac{t'+x}{t'-x}\right)\right] \\ & \times\exp\left[-\mathrm{i}\frac{k_n}{2}\ln\left(t'^2 - x^2\right)\right]\end{aligned} \tag{13}$$

with $t'(t) \equiv t - t_0 + \frac{L_0}{\nu}$, $0 < \nu < 1$. Figure 3 displays an exemplary plot of one specific such function. The



(a) Before reflection (b) During reflection (c) Redshifted wave packet (d) Late-time behavior (scale changed)

Fig. 4: Plots of $|\psi(x)|^2$ of a one-dimensional Gaussian wave packet redshifted upon reflection off a moving wall in flat space. The vertical bar in (a)–(c) represents the moving wall. The horizontal scaling in (d) differs from (a)–(c).



(a) Before reflection (b) During reflection (c) Reflected wave packet (d) Late-time behavior

Fig. 5: Plots of $|\psi(v)|^2$ of a one-dimensional Gaussian wave packet in an infinite square well in hyperbolic space.

solutions (13) are normalized to 1 with respect to the standard form of the KG-invariant scalar product,

$$\langle\psi_1|\psi_2\rangle = \mathrm{i}\int \mathrm{d}x\psi_1^*\overleftrightarrow{\partial_t}\psi_2. \tag{14}$$

Furthermore, the respective norms are preserved in hyperbolic as well as in flat space, and we can directly show for (13) that

$$\langle\Psi_n|\Psi_m\rangle = \delta_{nm}. \tag{15}$$

Numerical investigations. – We now investigate the properties of a relativistic quantum wave packet evolving according to (7), *i.e.*, $m=0$. A one-dimensional relativistic Gaussian wave packet

$$\Psi(t,x) = A\int_{-\infty}^{\infty} \mathrm{d}p\mathrm{e}^{-\frac{c^2(p-p_0)^2}{2}+\mathrm{i}(px-\omega t)} \tag{16}$$

composed out of positive frequencies $\omega=|p|$ will have a norm of one with respect to (14) if

$$A = \frac{c}{\sqrt{\pi}}\left(\mathrm{e}^{-c^2p_0^2}+\sqrt{\pi}p_0c\,\mathrm{erf}(p_0c)\right)^{-\frac{1}{2}}, \tag{17}$$

where erf denotes the error function. The wave packet (16) has constant norm (of approximately 1 if c is chosen small enough) with respect to (14) during its evolution in the moving-wall system, however its absolute width with respect to the x-coordinate will grow with each reflection off the moving wall, as the wave packet will go through successive *redshifts*. If a one-dimensional wave reflects off a wall which is moving away at a constant speed, it experiences a redshift given by

$$1+z = \frac{f_{\mathrm{ref}}}{f_{\mathrm{inc}}} = \gamma^2(1+\nu)^2 = \frac{1+\nu}{1-\nu} \equiv \Lambda(\nu)^2, \tag{18}$$

with $\gamma=(1-\nu^2)^{-\frac{1}{2}}$, *e.g.*, for $\nu=\frac{1}{2}$, the redshift is $1+z=3$. In terms of the relativistic Hamiltonian $H=\sqrt{\pi_x{}^2}$, where π_x denotes the momentum variable conjugate to x, the corresponding reflection of a classical massless particle in one dimension off a moving wall implies the relation

$$1+z = \frac{H_{\mathrm{ref}}}{H_{\mathrm{inc}}}, \tag{19}$$

which analogously simply states the relation of the energy H_{inc} of a photon before a bounce from a moving mirror to its energy H_{ref} afterwards. As a measure for the redshift, we employ the expectation value $\langle\hat{H}\rangle$, which we call the energy expectation value in the following. In order to avoid the square root in the reduced Hamiltonian (especially helpful in higher-dimensional cases), we adopt the two-component notation [8] for (1) by defining

$$\psi = \phi+\chi, \qquad \mathrm{i}\partial_t\psi = \phi-\chi \tag{20}$$

and adapt it to the massless case to obtain

$$\hat{H} = -\frac{\sigma_3+\mathrm{i}\sigma_2}{2}\Delta + \frac{\sigma_3-\mathrm{i}\sigma_2}{2}, \tag{21}$$

where σ_i are the Pauli matrices and where Δ is the Laplace operator in flat space, *i.e.*, $\Delta=\frac{\partial^2}{\partial x^2}$. Upon defining a two-component vector from the complex functions ϕ and χ according to

$$\Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix}, \tag{22}$$

eq. (14) is expressed through

$$\langle\Psi_1|\Psi_2\rangle = 2\int \mathrm{d}x\Psi_1^\dagger\sigma_3\Psi_2 \tag{23}$$

and the energy expectation value through

$$\langle\hat{H}\rangle = 2\int \mathrm{d}x\Psi^\dagger\sigma_3\hat{H}\Psi. \tag{24}$$

The two-component form (21) implies the expected expression

$$\langle \hat{H}^2 \rangle = 2 \int \mathrm{d}x \Psi^\dagger \sigma_3 \hat{H}^2 \Psi = -\mathrm{i} \int \mathrm{d}x \psi^* \overleftrightarrow{\partial_t} (\Delta \psi) \qquad (25)$$

for the expectation value of the squared Hamiltonian. Upon reflection off a moving wall in flat space, the wave packet loses energy into the wall, while its KG norm is preserved. See fig. 4 for an illustration of such a bounce, calculated by numerically solving the massless KG equation on the one hand in flat space with moving boundary conditions, and on the other hand an illustration of the corresponding evolution in hyperbolic space with static boundary conditions in fig. 5. Using (23), we can compute position expectation values according to

$$\langle \hat{x} \rangle = 2 \int \mathrm{d}x \Psi^\dagger \sigma_3 x \Psi = \mathrm{i} \int \mathrm{d}x x \psi^* \overleftrightarrow{\partial_t} \psi \qquad (26)$$

and analogously in hyperbolic space using (12). We remark however that, unlike the Hamiltonian and the momentum operator, the position operator in relativistic quantum mechanics generally mixes positive- and negative-frequency components of the wave packet [8]. The prescription (26) therefore has to be used with caution, but may serve as the intuitive measure for the "center of mass" of the wave packet. For details on localization of relativistic particles, we refer the reader to the investigations in [9,10].

Summary and conclusions. – Exact solutions of the Schrödinger and Klein-Gordon equations in a domain with time-dependent boundaries are difficult to obtain [3–5,7]. With this letter, we contribute an infinite set of orthogonal exact solutions to the one-dimensional Klein-Gordon equation in an infinite square well with one wall moving at a constant velocity, a side result of previous investigations concerning quantum billiards [11,12]. These solutions are obtained employing a simple transformation to hyperbolic space. We furthermore investigated numerically the properties of a massless relativistic wave packet bouncing off the moving walls in flat and in hyperbolic space, and observed the expected redshift. Although the scope of this article was intended to be limited to a domain with one wall moving at constant speed, it would nevertheless be of interest to generalize these results to domains with more arbitrarily moving walls.

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