Hidden freedom in the mode expansion on static spacetimes

Lissa de Souza Campos¹,² · Claudio Dappiaggi¹,² · Luca Sinibaldi¹,²

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Abstract

We review the construction of ground states focusing on a real scalar field whose dynamics is ruled by the Klein–Gordon equation on a large class of static spacetimes. As in the analysis of the classical equations of motion, when enough isometries are present, via a mode expansion the construction of two-point correlation functions boils down to solving a second order, ordinary differential equation on an interval of the real line. Using the language of Sturm–Liouville theory, most compelling is the scenario when one endpoint of such interval is classified as a limit circle, as it often happens when one is working on globally hyperbolic spacetimes with a timelike boundary. In this case, beyond initial data, one needs to specify a boundary condition both to have a well-defined classical dynamics and to select a corresponding ground state. Here, we take into account boundary conditions of Robin type by using well-known results from Sturm–Liouville theory, but we go beyond the existing literature by exploring an unnoticed freedom that emerges from the intrinsic arbitrariness of secondary solutions at a limit circle endpoint. Accordingly, we show that infinitely many one-parameter families of sensible dynamics are admissible. In other words, we emphasize that physical constraints guaranteeing the construction of ground states do not, in general, fix one such state unambiguously. In addition, we provide, in full detail, an example on (1 + 1)-half Minkowski spacetime to spell out the rationale in a specific scenario where analytic formulae can be obtained.

Keywords

Ground states · Robin Boundary conditions · Static spacetimes

Claudio Dappiaggi
claudio.dappiaggi@unipv.it

Lissa de Souza Campos
lissa.desouzacampos@unipv.it

Luca Sinibaldi
luca.sinibaldi01@universitadipavia.it

¹ Dipartimento di Fisica, Università di Pavia, Via Bassi 6, 27100 Pavia, Italy
² INFN, Sezione di Pavia, Via Bassi 6, 27100 Pavia, Italy
1 Introduction

Quantum field theory on curved spacetimes has lead to significant improvements in our understanding of different physical phenomena ranging from particle production in cosmology to Hawking radiation in black hole physics. In the analysis of the vast majority of the available models, the first step consists in constructing quantum states for the underlying free fields. Under the mild assumption that the correlation functions are Gaussian, this reduces to the identification of an on-shell two-point correlation function that has to abide to physically motivated constraints. The prime example in this direction is the Hadamard condition, which ensures not only that the quantum fluctuations of all observables are finite, but also that Wick-ordered fields can be constructed following a locally covariant scheme. In turn, it entails control of the underlying renormalization group and of interactions that are studied at a perturbative level. Yet, in many concrete scenarios one is limited to abstractly argue the existence of such distinguished two-point functions and an explicit construction is, at best, elusive.

Major improvements occur when one concentrates on static spacetimes $\mathcal{M} \simeq \mathbb{R} \times \Sigma$, regardless of whether they are globally hyperbolic or not. Let us consider, for simplicity, a free, scalar field $\Psi: \mathcal{M} \to \mathbb{R}$ that abides to the Klein–Gordon equation. By calling $t$ the time coordinate along $\mathbb{R}$, the latter simplifies to

$$\left(\frac{\partial^2}{\partial t^2} + K\right) \Psi = 0, \quad (1)$$

where $K$ is an elliptic, second order partial differential operator. The key rationale consists of reading $K$ as a symmetric operator on the Hilbert space $\mathcal{H} := L^2(\Sigma, d\mu_\Sigma)$ of square-integrable functions with respect to the measure $d\mu_\Sigma$ induced by the Lorentzian metric tensor of $\mathcal{M}$ on $\Sigma$. This leads to two notable advantages, one at a classical and one at a quantum level, as described next.

At a classical level, solutions of (1) can be constructed as follows. Since $K$ is a real and symmetric operator, it admits a non-necessarily unique self-adjoint extension
\( K \). Assuming, for convenience, that \( K \) has positive spectrum, and given initial data \((\Psi_0, \dot{\Psi}_0) \in C^\infty_0(\Sigma) \times C^\infty_0(\Sigma) \cap D(\widetilde{K}) \times D(\widetilde{K})\), for each \( t \in \mathbb{R} \) we have

\[
\Psi_t := \cos(\sqrt{\widetilde{K}} t) \Psi_0 + \frac{\sin(\sqrt{\widetilde{K}} t)}{\sqrt{\widetilde{K}}} \dot{\Psi}_0 \in \mathcal{H},
\]

where each term is well-defined using spectral calculus. Moreover, there exists a unique \( \Psi \in C^\infty(M) \) such that,

\[
\Psi|_{\Sigma_t} = \Psi_t \quad \text{and} \quad \nabla_n \Psi|_{\Sigma_t} = \dot{\Psi}_t,
\]

where \( \Sigma_t \equiv \{ t \} \times \Sigma, \ t \in \mathbb{R} \), while \( n \) is the unit vector field normal to \( \Sigma_t \).

If \((M, g)\) is a globally hyperbolic spacetime without boundary, then there exists a unique choice for \( K \) and the dynamics is therefore unambiguously determined \([1]\). On the contrary, if \( K \) has more than one self-adjoint extension, then multiple, physically non equivalent scenarios do exist. The latter is not a remote possibility: it occurs for example when \((M, g)\) is a globally hyperbolic spacetime with a timelike boundary, see \([2]\). In this case, using the language of boundary triples \([3]\), the infinite set of different choices of self-adjoint extensions for \( \widetilde{K} \) can be put in correspondence with the choice of a boundary condition for \((1)\). In addition, this class of backgrounds encompasses several physically interesting scenarios such as AdS spacetime, which have also been studied by Ishibashi and Wald in \([4]\). More precisely, in the latter reference, the authors focus their attention on the Klein–Gordon equation on an \( n \)-dimensional AdS spacetime. While they are interested in the self-adjoint extensions of their counterpart of the operator \( K \), in \([4, \text{Sect. 3}]\) they restrict their attention to a radial operator built out of \( K \) and they classify its self-adjoint extensions. This strategy discards a large class of self-adjoint extensions of \( K \), which are a priori physically sensible. As we shall argue in the following, such limitation can be overcome without discarding the advantages of working with a radial equation.

At a quantum level, the assumption that \((M, g)\) is static guarantees a considerable advantage: the existence of a ground state. Under the same premises as in the previous paragraphs, the associated two-point function \( \psi_2(t, x, t', x') \) can be constructed directly as the integral kernel of the operator \([5]\)

\[
e^{-i \sqrt{\widetilde{K}}(t-t')} \frac{1}{2\sqrt{\widetilde{K}}}.
\]

Observe that, if \( \dim M = 2 \) and if the operator \( \widetilde{K} \) possesses zero modes, then, whenever the constant time hypersurfaces in \( M \) are non compact, one should remove them in order to avoid infrared singularities. Yet, since this specific hurdle plays no rôle in our analysis, we shall not discuss it further. Furthermore, if the underlying background is a globally hyperbolic spacetime with or without timelike boundary, then ground states are of Hadamard form as a consequence of the results of \([6, 7]\).

While at this stage the analysis of a scalar quantum field theory on a static spacetime seems a rather well-understood problem, the drawback lies in two crucial details.
On the one hand, when non unique, an explicit construction and characterization of all self-adjoint extensions of $K$ in Eq. (1) is a daunting task. On the other hand, the quantitative evaluation of physical observables in concrete scenarios, such as on black hole spacetimes, requires a deeper and more hands on knowledge of the two-point function, far beyond the spectral level as per Eq. (3). To bypass this conceptual hurdle, it is customary to consider static backgrounds with a high degree of symmetry. Beyond reasons of mathematical simplicity, this class includes many physically relevant backgrounds, such as cosmic strings, black holes and asymptotically AdS spacetimes.

In this paper, we consider the class of $n$-dimensional static spacetimes $\mathcal{M}$ that are isometric either to

$$\mathbb{R} \times I, \text{ if } n = 2 \quad \text{or} \quad \mathbb{R} \times I \times \Sigma_{j}^{n-2}, \text{ if } n > 2,$$

where $I \subseteq \mathbb{R}$, and $\Sigma_{j}^{n-2}$ are Cauchy-complete, connected, $(n-2)$-dimensional Riemannian manifolds of constant sectional curvature $j$. The line element associated to the metric tensor on $\mathcal{M}$ reads

$$ds^2 = -f(r)dt^2 + h(r)dr^2 + r^2 d\Sigma_{j}^{n-2}(\varphi_1, \ldots, \varphi_{n-2}),$$

where $f$ and $h$ are suitable positive functions. Barring some technical aspects that will be specified in the next sections, we emphasize that a large class of spacetimes is characterized by the line-element above, including black hole backgrounds ranging from the three-dimensional static BTZ spacetime to the $n$-dimensional Schwarzschild or Schwarzschild-AdS spacetime.

On top of these manifolds, we consider a real, scalar field $\Psi$ whose dynamics is ruled by the Klein–Gordon equation, which, as before, can be written as per (1). With the construction of a quantum field theoretical framework in mind, we are interested in obtaining distinguished two-point functions that correspond to ground states. Although the procedure outlined above is applicable, especially when considering scenarios where boundary conditions needs to be imposed, it is common to follow a more computationally oriented approach that exploits the underlying symmetries. In the following, we sketch the steps usually followed in the literature in these scenarios. More details will be given in the next sections of this work.

1. Consider a solution of the Klein–Gordon equation on $(\mathcal{M}, g)$ assuming that it admits a mode expansion:

$$\Psi_{\omega \eta j}(t, r, \varphi_1, \ldots, \varphi_{n-2}) = e^{-i\omega t} R_{\omega \eta j}(r) Y_j(\varphi_1, \ldots, \varphi_{n-2}),$$

where $Y_j(\varphi_1, \ldots, \varphi_{n-2})$ are the eigenfunctions of the Laplace operator on $\Sigma_{j}^{n-2}$ whose corresponding eigenvalue is denoted by $\eta_j$, while $\omega \in \mathbb{R}$ plays the standard rôle of frequency.

2. The only unknown function $R_{\omega \eta j}$ can be shown to satisfy an eigenvalue equation $\mathbf{A} R_{\omega \eta j} = \lambda R_{\omega \eta j}$ where $\mathbf{A} \equiv \mathbf{A}_{\omega, j}$ is a second order differential operator in the radial coordinate $r$ whose domain is the interval $I$, here taken for definiteness as
Most notably $A$ can be written in the form of a possibly singular Sturm–Liouville operator, see [8], that depends explicitly both on $\omega$ and on $\eta_j$. Yet, in order to allow a smooth reading of the text, we resort to a slight abuse of notation avoiding to indicate explicitly the dependence on these parameters, hence using the symbol $A$.

Similarly to the rôle played by $K$ in Eq. (1), one reads $A$ as a symmetric operator on a space of square-integrable functions over the interval $I = (a, b)$.

Following von Neumann’s theory of deficiency indices [9], three options are possible. $A$ can admit just one self-adjoint extension, a one-parameter or a four-parameters family of self-adjoint extensions, identifying in the last two cases an element either of the Lie group $U(1)$ or $U(2)$. In most applications, the last option does not occur.

At this stage it is necessary to pause the description of the procedure to construct a two-point function and draw the attention to self-adjoint extensions. More precisely, from the viewpoint of the differential equation $A R_{\omega \eta j} = \lambda R_{\omega \eta j}$, the existence of such extensions can be inferred by looking at the behavior of solutions close to $a$ and $b$, the endpoints of the interval $I$. Henceforth, for definiteness, we focus on $a$. The general theory of Sturm–Liouville operators guarantees that, for any $\lambda \in \mathbb{C}$, there is always a distinguished function $u$, called principal solution. In Sect. 3 we dwell on the technical details of this concept. For now it suffices to say that $u$ tends to zero as $r \to a^+$ faster than any other solution that is linearly independent from it, and it is square-integrable in any neighborhood of the endpoint $a$. Notwithstanding, the existence of another solution, called secondary solution, that is linearly independent from $u$ and square-integrable in any neighborhood of $a$ depends on the differential problem at hand. If such a solution does not exist at both endpoints, then it happens that there is a unique self-adjoint extension for $A$, see [8]. More interesting is the scenario for which that is not the case for some value of $\lambda \in \mathbb{C}$, on account of the fact that if a secondary solution exists, then it is highly non unique.

The intrinsic arbitrariness of the secondary solution lies at the core of this work. Suppose there exists a secondary solution at $a$, but only the principal one at $b$. From the viewpoint of the Sturm–Liouville operator, the choice of a specific secondary solution at $a$ is irrelevant as its rôle lies only in establishing a one-to-one correspondence between self-adjoint extensions of $A$ and boundary conditions of Robin type, assigned at the endpoint $a$. These exhaust all possibilities at the level of the ordinary differential equation and therefore one can read the choice of two different secondary solutions as two different, albeit equivalent, ways to span the same space of boundary conditions and, consequently, of solutions of the underlying ordinary differential equation. Yet, in this scheme, one is tempted to forget that the class of all physically relevant boundary conditions is not tied only to the self-adjoint extensions of $A$, rather to those of the operator $K$ in Equation (1). A direct analysis using for example von Neumann theory of deficiency indices clearly unveils that there are apparently several more options available when working directly with $K$.

As an example in this direction, consider the three-dimensional half-Minkowski spacetime, namely $\mathcal{M} = \mathbb{R} \times [0, \infty) \times \mathbb{R}$ endowed with the standard Cartesian coordinates $(t, z, x)$. If, on top of $\mathcal{M}$ we consider a massless, real, scalar field $\Phi$, it...
descends that the role of $K$ is played by $\Delta$, the Laplace operator on $[0, \infty) \times \mathbb{R}$. Without entering at this stage in many technical details, one can show that, in order to select a self-adjoint extension of the Laplacian, it is necessary to impose a boundary condition at $z = 0$. Using for example the theory of boundary triples, see [3], but also [10], one can see that, among the infinite choices, one can require that $\Phi|_{z=0} = \alpha(x) \partial_z \Phi|_{z=0}$ where $\alpha$ is an arbitrary smooth function depending only on the spatial coordinate $x$ along the boundary. This generalized Robin boundary condition yields a well-defined classical and quantum field theory. Yet, if one works at the level of radial equation and hence with the operator $\mathbf{A}$, it is not clear whether it can be accounted for. As a matter of fact, one seems to be limited to the choice of boundary conditions for which the rôle of $\alpha(x)$ is played by a complex number. Hence, at first glance, it seems as if working at the level of radial equation forces us to consider only a limited number of self-adjoint extensions and hence to discard a class of physically admissible scenarios.

One of the main goals of this paper is to show that a way to circumvent this issue is to revisit the analysis of radial equations in the construction of a classical and of a quantum, free field theory, focusing on the choice of a secondary solution, while keeping Robin boundary conditions. We shall prove that this impacts significantly the analysis of the underlying scalar field and its choice is not moot as it might seem at first glance. More precisely one is able to codify at a covariant level a much larger class of admissible boundary conditions than just a one-parameter family as the standard analysis might suggest.

The physical relevance of choosing a secondary solution is clear when one constructs the two-point correlation function of the underlying ground state. Let us thus focus once more on the procedure we started sketching at Page 4 and let us state the subsequent steps, as follows.

5 Since the two-point correlation function $\psi_2$ obeys the Klein–Gordon equation, it is suitable to use the same mode expansion as for the construction of the solutions $\Psi$. This, together with the ansatz that only positive frequencies contribution are of relevance, identifies a ground state. On account of the large isometry group of the background, $\psi_2$ is completely determined up to a kernel along the radial direction.

6 As explained in Sect. 5, such kernel can be constructed using an algorithmic scheme once a self-adjoint extension for the operator $\mathbf{A}$ has been chosen in terms of a Robin boundary conditions imposed at the level of principal and secondary solutions.

We emphasize that the procedure 1–5 has been extensively applied on static space-times with a timelike boundary in the last years. To mention a few, exhaustive works based on von Neumann deficiency index theory are [4, 11], on AdS spacetimes, and [12], on a static BTZ black hole. Beyond these, analyses based on a mode expansion and on Robin boundary conditions and used in the construction of physically-sensible two-point functions within quantum field theory on asymptotically AdS spacetimes can be found in [13–17], and, more recently, also in [18–22].

The scope of this work is to highlight the fundamental rôle played, in this whole procedure, by the secondary solutions of the underlying Sturm–Liouville problem. To strengthen this statement we consider a simple, yet illustrative example, namely the two-dimensional half-Minkowksi spacetime $\mathbb{R} \times \mathbb{R}_+$. The advantage is that, in this scenario, we can address the problem using explicit, analytic formulae that allow to...
make clear that even minor adjustments to the choice of secondary solution yield, at
the fully covariant level, boundary conditions that have a completely different physical
interpretation. In a nutshell, we aim to convey that the choice of secondary solution is
of physical consequence.

This paper is organized as follows. In Sect. 2 we show that the Klein–Gordon equa-
tion untangles into a Sturm–Liouville problem for the radial part of the Klein–Gordon
operator on static spacetimes with maximally symmetric sections. Subsequently,
in Sect. 3 we provide straightforward generalizations of main results from singular
Sturm–Liouville theory that allow us to obtain all self-adjoint representations of the
latter. Markedly, singular endpoints give rise to an ambiguity in the definition itself
of generalized Robin boundary conditions. We clear up this ambiguity in Sect. 4 by
defining generalized \((\gamma, \nu)\)-Robin boundary conditions and explaining its connection
with the regular case. In Sect. 4.2 we show how a boundary condition on the radial
part translates to a boundary condition on the full solution \(\Psi\). Insofar as solutions
of the Klein–Gordon equation characterize a classical dynamics, it is meaningful
to include a discussion on the canonical quantization procedure. Hence, in Sect. 5
we explain the connection between the imposition of the canonical commutation
relations and the spectral resolution of the identity given by the before-mentioned
Sturm–Liouville problem. We illustrate the main points of this work in a detailed
example given in Sect. 6. Most importantly, this example clarifies in which sense the
generalized \((\gamma, \nu)\)-Robin boundary conditions imposed on the radial part may render
time-dependent boundary conditions on \(\Psi\). Final remarks are given in Sect. 7.

2 The Klein–Gordon equation

In this initial section we introduce both the geometric data of the spacetimes we are
interested in and the Klein–Gordon equation. In addition we show that, under the
specific assumptions on the background metric, the Klein–Gordon equation can be
reduced to a Sturm–Liouville problem.

In this work, for \(n > 2\), \(\Sigma_{j}^{n-2}\) denotes a Cauchy-complete, connected, \((n - 2)\)-
dimensional Riemannian manifold of constant sectional curvature \(j\), parametrized
by \((\varphi_1, \ldots, \varphi_{n-2})\), and whose standard metric has an associated line element
d\(d \Sigma_{j}^{n-2}(\varphi_1, \ldots, \varphi_{n-2})\). Unless stated otherwise, we shall assume \(j\) has been nor-
malized so that \(j \in \{-1, 0, +1\}\). The symbol \(\mathcal{M}\) refers to an \(n\)-dimensional, static
spacetime isometric to the warped geometry \(\mathbb{R} \times I \times \Sigma_j^{n-2}\), where \(I \subseteq \mathbb{R}\), while the
line element of the underlying metric read in global Schwarzschild-like coordinates
\((t, r, \varphi_1, \ldots, \varphi_{n-2})\):

\[ds^2 = - f(r)dt^2 + h(r)dr^2 + r^2d \Sigma_{j}^{n-2}(\varphi_1, \ldots, \varphi_{n-2}).\]  \(4\)

For convenience, we shall call \(t \in \mathbb{R}, r \in I \subseteq \mathbb{R},\) and \((\varphi_1, \ldots, \varphi_{n-2})\), respectively,
the time, the radial and the angular coordinates. Equation (4) is completely specified
aside from the two functions \(f, h\). For simplicity, we assumed them to be elements
of \(C^\infty(I; (0, \infty))\), although in many instances throughout this work less regularity
would suffice. Note that we also allow for the case \( n = 2 \), in which \( \mathcal{M} \) is isometric to \( \mathbb{R} \times I \) endowed with the line element \( ds^2 = -f(r)dt^2 + h(r)dr^2 \).

**Remark 1** We consider \( I \) to be an open interval, say \( I = (a, b) \), which might suggest that we are discarding scenarios of notable interest such as globally hyperbolic manifolds with timelike boundary, e.g. the universal cover of \( AdS_n \). In these cases, the counterpart of \( I \) would include one or both endpoints in the domain of the coordinate \( r \). Yet, if one is interested in the analysis of boundary conditions and their effects, it suffices to focus the attention on the interior of the underlying manifold. Therefore, our analyses can be straightforwardly applied to such cases as well.

On \( \mathcal{M} \), we consider a free, scalar field with mass \( m_0 \geq 0 \), whose dynamics is ruled by the Klein–Gordon equation:

\[
P\Psi := (\Box - m_0^2 - \xi R)\Psi = 0, \tag{5}
\]

where \( \xi \in \mathbb{R} \), while \( R \) is the scalar curvature built out of the metric as per Eq. (4). In the case in hand, the D’Alembert wave operator, denoted by \( \Box \), reads

\[
\Box = -\frac{1}{f(r)} \frac{d^2}{dr^2} + \frac{1}{h(r)} \frac{d}{dr} + \frac{\partial_r (f h r^{n-4})}{f h r^{n-2}} \partial_r + \frac{\Delta_{\Sigma_j}^{n-2}}{r^2},
\]

where \( \Delta_{\Sigma_j}^{n-2} \) is the Laplace operator on \( \Sigma_j^{n-2} \). In the following, we construct the solutions of the Klein–Gordon equation. Although (5) can be recast in the form of (1), we take a route aligned with the procedure \( \text{⃣}–\text{❼} \) described in the Introduction. Assuming that the regularity of \( \Psi \) is such that we can work at the level of modes, we consider the ansatz

\[
\Psi^{\omega\eta}_{\omega\eta j}(t, r, \varphi_1, \ldots, \varphi_{n-2}) = e^{-i\omega t} R^{\omega\eta j}(r) Y_j(\varphi_1, \ldots, \varphi_{n-2}), \tag{6}
\]

where \( Y_j(\varphi_1, \ldots, \varphi_{n-2}) \) are the eigenfunctions of \( \Delta_{\Sigma_j}^{n-2} \) with corresponding eigenvalues denoted by \( \eta_j \). Observe that \( \Delta_{\Sigma_j}^{n-2} \) has a continuous spectrum if \( j \in \{-1, 0\} \), while a discrete one if \( j = 1 \).

Equation (6) in combination with (5) yields that \( R^{\omega\eta j} \) obeys to a second-order, ordinary differential equation, dubbed radial equation:

\[
\mathbf{A} R^{\omega\eta j}(r) = 0
\]

\[
\mathbf{A} := \frac{d^2}{dr^2} + \left[ \frac{s(r)}{2} + \frac{n - 2}{r} \right] \frac{d}{dr} + \left[ \frac{\omega^2}{f(r)} + \frac{\eta_j}{r^2} - m_0^2 - \xi R \right] h(r), \tag{7}
\]

where \( s(r) := \frac{f'(r)}{f(r)} - \frac{h'(r)}{h(r)} \). We can rewrite (7) as

\[\Box \Psi = 0\]
\[(L - \lambda)R_{\text{even}}(r) = 0,\]
\[L := A + \lambda = \frac{1}{\mu(r)} \left( -\frac{d}{dr} \left( p(r) \frac{d}{dr} \right) + q(r) \right), \tag{8}\]

where
\[\lambda := \begin{cases} 
\omega^2, & \text{if } f(r) \neq 1, \\
\omega^2 - m_0^2 - \xi R, & \text{if } f(r) = 1 \text{ and } R \text{ is constant}, \\
\omega^2 - m_0^2, & \text{otherwise}. 
\end{cases} \tag{9}\]

If \(\lambda = \omega^2\), the functions \(p, q\) and \(\mu\) are given by
\[p(r) := r^{n-2} \sqrt{\frac{f(r)}{h(r)}} =: \frac{r^{2n-4}}{\mu(r)}, \tag{10a}\]
\[q(r) := r^{n-4} (\eta_j - r^2 (m_0^2 + \xi R)) \sqrt{f(r)h(r)}. \tag{10b}\]

In the remaining cases the corresponding expressions can be derived directly from Eq. (7), but we omit listing them as they are a rather straightforward modification of Eqs. (10a) and (10b). To conclude this section we observe that Eq. (7) identifies a, possibly singular, Sturm–Liouville problem, following the standard nomenclature of ordinary differential equations, see e.g. [8].

## 3 Self-adjoint extensions

In the construction of ground states for the Klein–Gordon field \(\Psi\), it is essential to build the advanced and retarded fundamental solutions associated to the operator \(P\) as in Equation (5). To this end we bear in mind a procedure that has been considered in several examples in the literature [15–20], mainly when the underlying spacetime possesses a conformal, timelike boundary. The starting point is \(A\), as per Equation (8), which shall be read as an operator on the Hilbert space \(L^2(I, \mu(r)dr)\).

The operator \(A\), and consequently also \(L\), is manifestly symmetric when taken with the dense domain \(C^\infty_0(I)\). Herein, we scrutinize whether \(L\) admits self-adjoint extensions and, if so, how many of them. This is a mathematical question that can be answered by combining tools of Sturm–Liouville theory with the theory of unbounded operators on Hilbert spaces, see e.g. [9]. Accordingly, in the following we recall the main results known in the literature that are of relevance to our investigation as well as necessary to make this work self-contained. All definitions and lemmas introduced here culminate in Theorem 3.5, which constitutes the resolution to the question in hand.

First, let us pose the question more precisely. Consider the Sturm–Liouville problem, as in (8),
\[LR(r) := \frac{1}{\mu(r)} \left( -\frac{d}{dr} \left( p(r) \frac{d}{dr} \right) + q(r) \right) R(r) = \lambda R(r), \tag{11}\]

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where as of now we omit the subscripts $\omega, \eta_j$ from the radial function for decluttering. In addition, letting $\mathcal{L}^1_{\text{loc}}$ refer to locally integrable functions, we assume that

$$1/p, q, \mu \in \mathcal{L}^1_{\text{loc}}(I), \quad \mu > 0, \quad \text{and} \quad r \in I := (a, b), \quad -\infty \leq a < b \leq \infty,$$

As alluded to in the previous paragraphs, $L$ as per Equation (11) identifies either a minimal or a maximal operator respectively indicated by $L_{\text{min}}$ and $L_{\text{max}}$, with corresponding domains

$$D_{\text{min}}(L_{\text{min}}) := \overline{C_0^\infty(I)},$$
$$D_{\text{max}}(L_{\text{max}}) := \{ y : I \to \mathbb{C} \mid p y' \in AC_{\text{loc}}(I), \text{ and } y, \mu^{-1}Ly \in L^2(I, \mu(r)dr) \},$$

where the closure is taken with respect to the graph topology, and $AC_{\text{loc}}(I)$ denotes the set of functions that are absolutely continuous on all compact intervals of $I$. Specifically, our goal is to find self-adjoint extensions $L_{\text{S.A.}}$ of $L_{\text{min}}$, $L_{\text{min}} \subset L_{\text{S.A.}} = L^*_{\text{S.A.}} \subset L_{\text{max}}$, whose domain shall be denoted by $D_{\text{S.A.}}(L_{\text{S.A.}})$. If their spectrum satisfies $\sigma(L_{\text{S.A.}}) \subseteq [0, \infty)$, then we say $L_{\text{S.A.}}$ is a positive, self-adjoint extension of $L_{\text{min}}$.

In order to reach the goal stated above, we introduce some additional tools tailoring the analysis of [8] to the case of interest, i.e. Eq. (11) together with the assumptions of the previous sections.

For $y, z \in AC_{\text{loc}}(I)$ we denote the Lagrange sesquilinear form and the Wronskian, respectively, by

$$[y, z] := p(y\overline{z}' - y'\overline{z}) = -[z, y], \quad (12)$$
$$\{y, z\} := p(yz' - y'z) = [y, z]. \quad (13)$$

**Definition 3.1** Let $e$ be an endpoint of the interval $I = (a, b)$, i.e. $e \in \{a, b\}$. Define $I_c := (a, c)$ if $e = a$, while $I_c := (c, b)$ if $e = b$. We say the endpoint $e$ is

(i) regular if $1/p, q, \mu \in L^1(I_c)$ for some (and hence any) $c \in I$;
(ii) singular if it is not regular;
(iii) limit circle if all solutions of (11) lie in $L^2(I_c, \mu(r)dr), \forall c \in I$;
(iv) limit point if it is not limit circle.

The following definition is especially relevant for our analysis since it differentiates among the solutions of Equation (11) depending on their behaviour close to an endpoint.

**Definition 3.2** Let $y$ be a non-vanishing solution of (11) in $I_c, \forall c \in I$. Then we say $y$ is a

(i) principal solution at $e$ if, for any other solution $z$ of Eq. (11) that is linearly-independent from $y$,

$$\frac{y(x)}{z(x)} \xrightarrow{x \to e} 0.$$
(ii) secondary (or non-principal) solution at $e$ if it is not a principal solution.

Definitions 3.1 and 3.2 relate by the fact that at a limit point only the principal solution belongs to $L^2(I_c, \mu(r)dr)$. Manifestly, the classification given by Definition 3.2 is of relevance only when at least one of the endpoints is a limit circle. Thus, for the remainder of this section, we assume that on $I = (a, b)$, $a$ is a limit circle while $b$ is a limit point. In addition, we denote by $u$ and $v$, respectively, the principal and secondary solutions at the limit circle endpoint and we set $[u, v](c) := \Lambda_1 \neq 0$ for all $c \in I$. We observe that although $a$ and $b$ might be singular endpoints, for any $y, z \in D_{\max}(L_{\max})$, since the following limits exist, it makes sense to define

$$[y, z](a) := \lim_{r \to a^+} [y, z] < \infty \quad \text{and} \quad [y, z](b) := \lim_{r \to b^-} [y, z] < \infty. \quad (14)$$

Next, we report three results concerning the interplay between the Lagrange sesquilinear form and Eq. (11). Their proofs, omitted here, are a direct adaptation to the case in hand respectively of Lemmas 10.4.1, 10.4.2 and 10.4.6 in [8].

**Lemma 3.1** Let $L$ be as per Eq. (11) and let $c, d \in I$. Given $\alpha, \beta, \gamma, \delta \in \mathbb{C}$, there exists $y \in D_{\max}(L_{\max})$ such that

$$y(c) = \alpha, \quad y(d) = \gamma,
\quad (py')(c) = \beta, \quad (py')(d) = \delta.$$\hspace{1cm} (15)

**Lemma 3.2** (Lagrange bracket decomposition) Let $L$ be as per Eq. (11) and let $u, v$ be any two solutions lying in $D_{\max}(L_{\max})$ such that $[u, v](c) = \Lambda \neq 0$ for all $c \in [a, b]$. It holds that, for all $y, z \in D_{\max}(L_{\max})$

$$[y, z](c) = -\overline{\Lambda}^{-1} \{ [y, v](c)[\overline{z}, u](c) - [y, u](c)[\overline{z}, v](c) \}.$$\hspace{1cm} (16)

**Lemma 3.3** Let $L$ be as per Eq. (11). Then for any $\lambda \in \mathbb{R}$ and $\alpha, \beta \in \mathbb{C}$, there exists $f \in D_{\max}(L_{\max})$ such that

$$[f, u](a) = \alpha, \quad [f, v](a) = \beta.$$\hspace{1cm} (17)

Moreover, if $a$ is a regular endpoint, then there exists $g \in D_{\max}(L_{\max})$ such that

$$g(a) = \alpha, \quad pg'(a) = \beta.$$\hspace{1cm} (18)

**Remark 2** It is interesting to notice that if $\Lambda = 1$, (16) follows directly from (15) by setting $g = f$. This is not the case if $\Lambda \neq 1$ and this plays a significant part in the discussion of generalized versus regular boundary conditions in the next sections.

The following result concerns properties of the self-adjoint extensions of $L_{\min}$, whereas their existence is a direct consequence of von Neumann lemma [9, Thm.5.43] since the differential operator $L$ in Eq. (10a) has real coefficients. For its proof we refer to [8, Th. 10.4.1], and references therein.
Lemma 3.4 If $L_{S.A.}$ is a self-adjoint extension of $L_{min}$, then there exists $g \in D_{S.A.}(L_{S.A.}) \subset D_{max}(L_{max})$ such that

1) $g \notin D_{min}(L_{min})$ and $[g, g](a) = 0$;
2) $D_{S.A.}(L_{S.A.}) = \{ f \in D_{max}(L_{max}) : [f, g](a) = 0 \}$.

Conversely, for any $g \in D_{max}(L_{max})$ abiding to the conditions in item (1), there exists a self-adjoint extension of $L_{min}$ whose domain $D_{S.A.}(L_{S.A.})$ is defined as per item (2).

Our goal is reached thanks to the following result, which is specially tailored to befit singular Sturm–Liouville problems. In particular, it is instrumental to relating the existence of multiple self-adjoint extensions to the choice of specific boundary conditions. We include a detailed proof due to its relevance and in light of the fact that it is not exactly the well-known result as per [8, Thm. 10.4.5], but rather a slight generalization of it. Namely, the principal and secondary solutions are not necessarily normalized to $[u, v] = 1$.

Theorem 3.5 Let $L$ be as in (11). As per Definition 3.2, let $u$ and $v$ be principal and secondary real-valued solutions at $r = a$ such that $[u, v] = \Lambda \neq 0$. Then for any $(B_1, B_2) \in \mathbb{R}^2 \setminus \{(0, 0)\}$,

$$D_{S.A.}(L_{S.A.}) = \{ y \in D_{max}(L_{max}) : B_1[y, u](a) + B_2[y, v](a) = 0 \} \quad (17)$$

is the domain of a self-adjoint extension of $L_{min}$. Moreover, all self-adjoint extensions of $L_{min}$ are of this form.

Proof We divide the analysis in two separate parts: proof of the first statement, and proof of the “moreover” statement.

Part 1.

Let $(B_1, B_2) \in \mathbb{R}^2 \setminus \{(0, 0)\}$. To prove that (17) is the domain of a self-adjoint extension of $L_{min}$, we shall use Lemma 3.4. In other words we set $g = \frac{B_1 u + B_2 v}{\Lambda}$ and, using Lemma 3.1, we can make sure that $g, u, v \in D_{max}(L_{max})\setminus D_{min}(L_{min})$. It descends

$$[g, g](a) = \frac{1}{\Lambda} (B_1 [g, u](a) + B_2 [g, v](a)) = 0,$$

$$[g, u](a) = -B_2 \quad \text{and} \quad [g, v](a) = B_1.$$

Observe that item (2) of Lemma 3.4 is automatically fulfilled by (17).

Part 2.

Consider now $L_{S.A.}$ a self-adjoint extension of $L_{min}$. By Lemma 3.2, for $y, g \in D_{max}(L_{max})$, it holds

$$[y, g](a) = -\frac{1}{\Lambda} [[y, v](a) [\overline{g}, u](a) - [y, \overline{u}](a) [\overline{g}, v](a)]$$

$$= -\frac{1}{\Lambda} \left[ [y, v](a) C_1 - [y, \overline{u}](a) C_2 \right],$$
where $C_1 := [\bar{g}, \bar{u}](a)$ and $C_2 := [\bar{g}, v](a)$. On account of Lemma 3.4 there exists $g \notin D_{\min}(L_{\min})$ such that $[g, g](a) = 0$. By setting $y = g$ in the equation displayed above and assuming both $u$ and $v$ to be real-valued, it descends

$$[g, g](a) = -\frac{1}{\Lambda} \{[g, v](a) C_1 - [g, u](a) C_2\} = -\frac{1}{\Lambda} \{C_2 C_1 - \bar{C}_1 C_2\}.$$ 

Thus

$$[g, g](a) = 0 \iff C_1 C_2 \in \mathbb{R}.$$ 

In addition, still Lemma 3.4 guarantees that $f \in D_{S.A.}(L_{S.A.})$ if and only if $[f, g](a) = 0$. This reduces to (17) setting therein $B_1 = C_1 C_1$ and $B_2 = C_1 C_2$.

**Remark 3** Note that the proof of Theorem 3.5 assuming $[u, v] = \Lambda \neq 0$ is analogous to that on [8, Thm. 10.4.5] that assumes $[u, v] = 1$. It is worth mentioning that this normalization does not select a secondary solution. It is easy to see that this is the case if we take into account that $[u, u] = 0$ for real-valued $u$. In turn, the reality of both $u$ and $v$ is an essential aspect of the validity of the proof. In addition, a consequence of this restriction is that (17) can be equivalently written in terms of the Wronskians instead of the Lagrange sesquilinear form, i.e.

$$B_1 \{y, u\}(a) + B_2 \{y, v\}(a) = 0.$$

To summarize, Theorem 3.5 characterizes all self-adjoint realizations of the Sturm–Liouville problem under consideration. Namely, $L_{S,A} y = L_{S,A}^* y$ for $y \in L^2(I_c, \mu(r)dr)$ such that

$$B_1 \{y, u\}(a) + B_2 \{y, v\}(a) = 0 \text{ for } (B_1, B_2) \in \mathbb{R}^2 \setminus \{(0, 0)\}.$$ 

**4 Generalized $(\gamma, \nu)$-Robin boundary conditions**

In this section we take a closer look at the boundary condition stated in (17) and we reiterate two important facts:

- although (17) depends on the choice of the pair $(B_1, B_2) \neq (0, 0)$, it is always possible to rescale $y \in D_{\max}(L_{\max})$ so to fix one of the parameters to 1, i.e. we can consider only pairs of the form $(1, \frac{B_2}{B_1})$;
- the characterization of $D_{S,A.}(L_{S,A.})$ also depends on the chosen secondary solution.

At the mere level of the Sturm–Liouville problem under consideration, the freedom in the choice of secondary solution is inconsequential if one is interested in characterizing all self-adjoint extensions of the corresponding operator. Notwithstanding, it plays a distinguished, physically relevant rôle when we turn back to analyzing the dynamics of the Klein–Gordon field ruled by Eq. (5). The following definitions aim at highlighting this freedom in the overall process and the difference that occurs when considering a singular rather than a regular Sturm–Liouville problem.
Definition 4.1 (Regular $\gamma$-Robin boundary condition) Let $L$ be as per (11). Given any self-adjoint realization $L_{S.A.}$, we say that $y \in D_{S.A.}(L_{S.A.})$ satisfies a regular $\gamma$-Robin boundary condition at $a$ if

$$\lim_{r \to a} \{\cos(\gamma) y + \sin(\gamma) y'\} = 0 \quad \text{for} \quad \gamma \in [0, \pi),$$

where the prime indicates the derivative along the $r$-direction. In particular, we say that $y$ abides to a

1. regular Dirichlet boundary condition at $a$ if it satisfies a regular $0$-Robin boundary condition:

$$\lim_{r \to a} y = 0 \quad \text{and} \quad \lim_{r \to a} y' = c \in \mathbb{R}.$$

2. regular Neumann boundary condition at $a$ if it satisfies a regular $\frac{\pi}{2}$-Robin boundary condition:

$$\lim_{r \to a} y' = 0 \quad \text{and} \quad \lim_{r \to a} y = c \in \mathbb{R}.$$

Definition 4.2 (Generalized $(\gamma, v)$-Robin boundary condition) Let $L$ be as per (11) and let $u$ be the principal solution at $a$ and $v$ any secondary solution at $a$, real-valued and such that $\{u, v\} = \Lambda$. Given any self-adjoint realization $L_{S.A.}$, we say that $y \in D_{S.A.}(L_{S.A.})$ satisfies a generalized $(\gamma, v)$-Robin boundary condition at $a$ if

$$\lim_{r \to a} \{\cos(\gamma)\{y, u\} + \sin(\gamma)\{y, v\}\} = 0 \quad \text{for} \quad \gamma \in [0, \pi). \quad (18)$$

In particular, we say that $y$ abides to a

1. generalized Dirichlet boundary condition at $a$ if it satisfies a generalized $(0, v)$-Robin boundary condition:

$$\lim_{r \to a} \{y, u\} = 0. \quad (19)$$

2. generalized $v$-Neumann boundary condition at $a$ if it satisfies a generalized $(\frac{\pi}{2}, v)$-Robin boundary condition:

$$\lim_{r \to a} \{y, v\} = 0. \quad (20)$$

It is worth stressing that Definition 4.1 is applicable only to regular Sturm–Liouville problems since it implicitly requires differentiability of the solution at the endpoint $a$. In addition, consistently with what one could a priori expect, the “Dirichlet boundary condition” is actually independent of the choice of the secondary solution. In the following, we elucidate more in detail the connection between the two definitions above.

4.1 Reduction to the regular case

Consider the setting of Theorem 3.5, and assume that $r = a$ is a regular endpoint as per Definition 3.1. For real-valued $u$ and $v$ such that $\{u, v\} = \Lambda$, a solution $y =$
cos(γ)u + sin(γ)v ∈ L^2(I, μ(r)dr) satisfies a generalized (γ, v)-Robin boundary condition, as per (18). Hence

\[ [y, u](a) = -\Lambda \sin(γ), \quad [y, v](a) = \Lambda \cos(γ). \]  

(21)

On account of Lemma 3.3, since \( a \) is a regular endpoint, if we choose \( u \) and \( v \) such that

\[ u(a) = 0 \quad \text{and} \quad (pv')(a) = 0, \]

then (21) implies that

\[ y(a) = -\frac{\Lambda \sin(γ)}{pu'(a)} \quad \text{and} \quad y'(a) = -\frac{\Lambda \cos(γ)}{pv(a)}. \]

Hence

\[ \cos(γ)y(a) + \sin(γ)y'(a) = \]

\[ = -\frac{\Lambda \sin(γ) \cos(γ)}{p} \left( \frac{1}{u'(a)} + \frac{1}{v(a)} \right) = 0 \iff v(a) = -u'(a). \]

That is, at a regular endpoint, for a given \( u \) there is a choice of secondary solution \( v \) for which the generalized \((γ, v)\)-Robin boundary condition, as per Definition 4.2, yields a regular \( γ \)-Robin boundary condition, as per Definition 4.1. Conversely, if we do not choose it in such a way and if \( γ \neq 0 \), then a generalized boundary condition does not necessarily reduce to a regular one.

### 4.2 Generalized \((γ, v)\)-Robin boundary conditions and the Klein–Gordon equation

In view of the foregoing discussion, it is natural to wonder what is the consequence of choosing a specific generalized \((γ, v)\)-Robin boundary condition at the level of the fully covariant Klein–Gordon equation. This question becomes especially relevant when we are working on a globally hyperbolic spacetime with timelike boundary [2], such as the Poincaré patch of an \( n \)-dimensional anti-de Sitter spacetime (PAdS\( _n \)). In this case, it is known that the dynamics is completely specified when, and only when, initial data are supplemented with a boundary condition assigned at conformal infinity. Then, one would slavishly follow the analysis outlined in the previous sections.

For definiteness, let us assume we are working under conditions for which Definition 4.2 is meaningful. Explicitly, take \( Ψ \) to be a solution of the Klein–Gordon Eq. (5) written as the mode expansion given in (6). In addition, let \( u \) and \( v \) be real-valued principal and secondary solutions at an endpoint \( a \) for the radial equation, such that the radial mode satisfies a generalized \((γ, v)\)-Robin boundary condition. One can infer that the latter translates to a boundary condition on \( Ψ \):

\[ \cos(γ)\{Ψ, \tilde{u}\}(a) + \sin(γ)\{Ψ, \tilde{v}\}(a) = 0, \]

(22)
where
\[ \tilde{u} = \int_{\sigma(\Delta_j^{n-2})} d\mu(\Sigma_j^{n-2}) \int_{\sigma(A)} d\lambda \, e^{-i\sqrt{\lambda}t} u_j(r_1, \ldots, \varphi_{n-2}), \]
\[ \tilde{v} = \int_{\sigma(\Delta_j^{n-2})} d\mu(\Sigma_j^{n-2}) \int_{\sigma(A)} d\lambda \, e^{-i\sqrt{\lambda}t} v_j(r_1, \ldots, \varphi_{n-2}), \]

where \( \int_{\sigma(\Delta_j^{n-2})} d\mu(\Sigma_j^{n-2}) \) is the integral over the spectrum of the Laplace operator on \( \Sigma_j^{n-2} \). Details regarding the latter are left to the reader since they play no rôle in our discussion, yet we observe that if \( j = 1 \) this integral reduces to a sum of (hyper-)spherical harmonics, whereas if \( j \in \{0, 1\} \) it is nothing but an ordinary Lesbegue integral. Similarly, \( \int_{\sigma(A)} d\lambda \) is formally the integral over the spectrum of the self-adjoint extension \( A \) with respect to the associated spectral measure. For all practical purposes in many instances \( \sigma(A) = (0, \infty) \) and the integral reduces to a standard Lesbegue integration on the half real line.

With the discussion of Sect. 4 in mind, we see that (22) reduces to a regular Robin boundary condition only under special conditions. In addition, we highlight that generalized \((\gamma, v)\)-Robin boundary conditions on \( R(r) \) translate at the level of the Klein–Gordon equation, to a wide variety of boundary conditions, including time-dependent ones. Although at this stage, this statement might be elusive and hidden in the meanders of (22), it is manifest in the concrete example thoroughly discussed in Sect. 6.2.

5 The quantum dynamics

The analysis of the classical solutions to the Klein–Gordon equation is just the starting point to obtain a full-fledged, covariant quantization framework. In this paper we shall not give all the details of the latter, see [15–20], rather we focus on the construction of ground states admitting generalized \((\gamma, v)\)-Robin boundary conditions.

**Definition 5.1** Let \( \mathcal{M} \) and \( P \) be as defined in Sect. 2. A two-point function of a quantum state is a bidistribution \( \psi_2 \in \mathcal{D}'(\mathcal{M} \times \mathcal{M}) \) such that

1. it solves the Klein–Gordon equation in both entries:
   \[ (P \otimes 1)\psi_2 = (1 \otimes P)\psi_2 = 0; \]
2. it satisfies the canonical commutation relations:
   \[ E(f, f') := \psi_2(f, f') - \psi_2(f', f), \quad \forall f, f' \in C_0^\infty(M), \]
   where \( E \) is the advanced minus retarded fundamental solution associated to \( P \);
3. it is positive:
   \[ \frac{1}{4} |E(f, f')|^2 \leq \psi_2(f, f)\psi_2(f', f') \quad \forall f, f' \in C_0^\infty(M). \]
In turn, the bi-distribution $E \in D'(\mathcal{M} \times \mathcal{M})$ is a solution of the initial value problem:

\[
(P \otimes \mathbb{1})E = (\mathbb{1} \otimes P)E = 0, \tag{23a}
\]
\[
E|_{\Sigma_t \times \Sigma_t} = 0 \text{ and } \nabla_\xi E|_{\Sigma_t \times \Sigma_t} = \delta_{\Sigma_t}, \tag{23b}
\]

where $\Sigma_t$ is any constant-time hypersurface, while $\delta_{\Sigma}$ is the Dirac delta thereon. It is important to stress that $E$ is a priori not unique, depending both on the underlying geometry and on the parameters $\xi$ and $m_0$ of the Klein–Gordon equation, see (5). The details for its construction using tools of Sturm–Liouville and spectral theories can be found in [23] and references therein.

As detailed in [23, Ch.2] and hinted at in the Introduction, among the plethora of two-point functions on a spacetime admitting Schwarzschild-like coordinates, as per (4), one can always distinguish the ones that characterize ground states. They are of the form

\[
\psi_2(x, x') = \lim_{\varepsilon \to 0^+} \int_{\sigma(\Delta_j)} d\eta \int_{\mathbb{R}} d\omega \Theta(\omega)e^{-i\omega(t-t'-i\varepsilon)}\tilde{\psi}_2(r, r')Y_j(\theta)\overline{Y_j(\theta')}, \tag{24}
\]

where $\Theta$ denotes the Heaviside step function and, for compactness, we have introduced the notation $\theta = (\varphi_1, \ldots, \varphi_{n-2})$. Using (23a) in combination with the canonical commutation relations in Definition 5.1 and with the completeness of the eigenfunctions of the Laplace operator $\Delta_{\Sigma_j}$, it turns out that the unknown $\tilde{\psi}_2(r, r')$ can be obtained by the spectral resolution of the Green function $G(r, r')$ associated to (7), see [24, Ch.7]. Namely, promoting $\lambda$ to a complex variable, one make use of the chain of identities

\[
\int_{\mathbb{R}} \omega d\omega \tilde{\psi}_2(r, r') = \frac{\delta(r - r')}{\mu(r)} = -\frac{1}{2\pi i} \oint_{C^\infty} d\lambda G(r, r'), \tag{25}
\]

where $C^\infty$ is an infinitely large circle in the $\lambda$-plane with a counter-clockwise orientation.

**Remark 4** Each generalized $(\gamma, v)$-Robin boundary condition on the radial mode $R(r)$ yields a different Green function $G(r, r')$ for the radial equation and, consequently, a different two-point function—a different ground state.

In the next section we give a neat and tangible example that unveils how the choice of different secondary solutions, even with the same value of $\gamma$, yields well-defined but inequivalent ground states. It corroborates our statement that, in a system where states can be constructed following a mode decomposition, the choice of a secondary solution for the radial equation remains free even after imposing all the physical constraints necessary to guarantee a sensible framework.

### 6 An illustrative example: the wave equation on $\mathbb{R} \times \mathbb{R}_+$

In this section, we outline a simple yet most illustrative example aimed at highlighting the relevance of the generalized $(\gamma, v)$-Robin boundary conditions: a real, scalar field
on the 2-dimensional half-Minkowski spacetime \( \mathbb{R} \times \mathbb{R}_+ \). There are two essential points to be taken into account with care.

- The endpoints to be considered in the corresponding Sturm–Liouville problem are regular, since the underlying manifold is globally hyperbolic with a timelike boundary, yet it is conceivable to impose thereon generalized \((\gamma, v)\)-Robin boundary conditions.
- The two-point functions for a massless scalar field on a two-dimensional background are ill-defined due to an infrared divergence, as implicitly pointed out in the Introduction, see Page 3. Yet, at the level of radial equation, since it does make sense to consider a massless field we shall explicitly write down the expressions for the green functions in this simplified scenario. This example allow us to see clearly the different behavior of the generalized \((\gamma, v)\)-Robin boundary conditions.

In standard Cartesian coordinates \((t, x, y)\), for \(t, y \in \mathbb{R}\) and \(x \in (0, \infty)\), the mode decomposition ansatz as per (6) reads

\[
\Psi_\omega(t, x) = e^{-i\omega t} \psi_\omega(x),
\]

where \(\psi_\omega(x)\) is nothing but a harmonic oscillator on the half-line:

\[
d^2\psi(x) dx^2 = -q^2 \psi(x), \quad \forall x \in (0, \infty),
\]

and \(q^2 \equiv \omega^2 - m_0^2\). Consider the basis of solutions given by

\[
y_1(x) := e^{+iqx} \quad \text{and} \quad y_2(x) := e^{-iqx}.
\]

As functions of \(x\) and considering \(q\) a possibly complex parameter, it follows that \(y_1(x)\) and \(y_2(x)\) are not square-integrable at \(x = \infty\) unless \(\text{Im}(q) > 0\) and \(\text{Im}(q) < 0\), respectively. Therefore, as per Definition 3.1, this endpoint is a limit point and the most general square-integrable solution therein can be written concisely as

\[
\psi_\infty(x) = y_1(x) \Theta(\text{Im}(q)) + y_2(x) \Theta(-\text{Im}(q)). \tag{26}
\]

Both \(y_1(x)\) and \(y_2(x)\) are square-integrable in a neighborhood of \(x = 0\). Still according to Definition 3.1, \(x = 0\) is a limit circle.

Using the nomenclature of Definition 3.2, the principal solution reads

\[
u(x) = \frac{y_1(x) - y_2(x)}{2i} = \sin(qx).
\]

As a secondary solution at \(x = 0\), we shall consider three possible choices:

\[
v_1 = \omega \frac{y_1(x) + y_2(x)}{2} = q \cos(qx),
\]
\[ v_2 = \frac{y_1(x) + y_2(x)}{2} = \cos(q x), \]

\[ v_3 = \frac{y_1(x) + y_2(x)}{2} + \frac{y_1(x) - y_2(x)}{2i} = \cos(q x) + \sin(q x). \]

For convenience, define \( s := \text{sign}(\text{Im}(q)) \), \( \text{Im}(q) \neq 0 \). We can write \( \psi_{\infty} \) in terms of the principal and secondary solutions as

\[ \psi_{\infty}(x) = a_{\kappa} u + b_{\kappa} v_{\kappa}, \]

where \( a_1 = a_2 = a_3 + 1 = i s \) and \( q b_1 = b_2 = b_3 = 1 \). Note that \( \psi_{\infty}(x) \) itself is independent of \( \kappa \). In addition, the solution

\[ \psi_{\kappa}(x) = \cos(\gamma) u(x) + \sin(\gamma) v_{\kappa}(x), \quad \text{for } \kappa \in \{1, 2, 3\}, \gamma \in \mathbb{R}, \quad (27) \]

satisfies a generalized \((\gamma, v_{\kappa})\)-Robin boundary condition at \( x = 0 \), i.e.

\[ \lim_{x \to 0} \{\cos(\gamma)\{\psi_{\kappa}, u\} + \sin(\gamma)\{\psi_{\kappa}, v_{\kappa}\}\} = 0. \]

### 6.1 Generalized versus regular Robin boundary conditions

Since the limits of \( y_1, y_2 \) and of their derivatives exist as \( x \to 0 \), we can cast the generalized \((\gamma, v_{\kappa})\)-Robin boundary condition above as a regular \( \gamma \)-Robin boundary condition:

\[ \lim_{x \to 0} \left( \psi_{\kappa} - \frac{1}{\beta_{\kappa}} \psi_{\kappa}' \right) = 0, \quad \text{for } \beta_{\kappa} = \frac{\cos(\gamma) u'(0) + \sin(\gamma) v_{\kappa}'(0)}{\cos(\gamma) u(0) + \sin(\gamma) v_{\kappa}(0)}. \quad (28) \]

We find that

\[ \beta_1 = \cot(\gamma), \quad (29a) \]
\[ \beta_2 = q \cot(\gamma), \quad (29b) \]
\[ \beta_3 = q (\cot(\gamma) + 1), \quad (29c) \]

which highlights the difference between a generalized and a regular Robin boundary condition. Markedly, in the regular scenario we can choose a secondary solution based on the property of obtaining a frequency-independent parameter \( \beta_{\kappa} \); in this case, \( \beta_1 \). Yet, frequency-dependent boundary conditions are also of physical relevance and hence there is no a priori reason to discard them. We emphasize that the main point of this work is not to introduce frequency-dependent boundary conditions, but rather to highlight the fact that frequency-dependent boundary conditions are already taken into account using the standard prescription of obtaining self-adjoint extensions of the spatial part of the Klein–Gordon operator. Manifestly, when the endpoint at which we are applying the boundary condition is singular, Equations (28) and (29) are meaningless.
6.2 Time-dependence of the boundary conditions

Analogously to the discussion in Sect. 4.2, given a radial solution of the wave function that satisfies a generalized \((\gamma, v_{\kappa})\)-Robin boundary condition, it is legitimate to wonder which is the corresponding boundary condition satisfied by the solution of the wave equation on \(\mathbb{R} \times \mathbb{R}_+\). For \(\psi_{\kappa}\) given by (27), let us consider a general solution:

\[
\Psi_{\kappa}(t, x, y) = \int d\omega e^{-i\omega t} \psi_{\kappa}(x).
\]

It can be written as

\[
\Psi_{\kappa}(t, x, y) = \cos(\gamma) \hat{u} + \sin(\gamma) \hat{v}_{\kappa},
\]

where, with a slight abuse of notation, we have denoted the Fourier transform with a hat. For the sake of clarity, let us consider the simplified scenario of \(m_0 = 0\). In this case we may compute explicitly the Fourier transforms indicated in equation above and we find

\[
\begin{align*}
\hat{u} &= i\pi(\delta(t + x) - \delta(t - x)), \\
\hat{v}_1 &= i\pi(\delta'(t + x) + \delta'(t - x)) \\
\hat{v}_2 &= \pi(\delta(t + x) + \delta(t - x)) \\
\hat{v}_3 &= \pi((1 + i)\delta(t + x) + (1 - i)\delta(t - x)).
\end{align*}
\]

We can now read which boundary condition is satisfied by \(\Psi_{\kappa}(t, x)\) at \(x = 0\) for each \(\kappa\). Formally, working at the level of distributions, we look for operators such that

\[
\begin{align*}
\lim_{x \to 0} (c_1 \Psi_1(t, x) + \partial_x \Psi_1(t, x)) &= 2i\pi \delta'(t)(c_1 \sin(\gamma) + \cos(\gamma)) = 0; \\
\lim_{x \to 0} (c_2 \Psi_2(t, x) + \partial_x \Psi_2(t, x)) &= 2i\pi (c_2 \delta(t) \sin(\gamma) + i\delta'(t) \cos(\gamma)) = 0; \\
\lim_{x \to 0} (c_3 \Psi_3(t, x) + \partial_x \Psi_3(t, x)) &= 2\pi (c_3 \delta(t) \sin(\gamma) + i\delta'(t)(\cos(\gamma) + \sin(\gamma)) = 0.
\end{align*}
\]

The above are satisfied if we take \(c_{\kappa}\) and \(\zeta_{\kappa}\) as

\[
\begin{align*}
c_1 &= 1, \\
c_2 &= -i \cot(\gamma) \partial_t =: \zeta_2 \partial_t, \\
c_3 &= -i \cot(\gamma)(1 + \tan(\gamma)) \partial_t =: \zeta_3 \partial_t.
\end{align*}
\]

Accordingly, the solution \(\Psi_{\kappa}(t, x)\) satisfies, for \(\kappa \in \{2, 3\}\):

\[
\lim_{x \to 0} (\zeta_{\kappa} \partial_t \Psi_{\kappa}(t, x) + \partial_x \Psi_{\kappa}(t, x)) = 0.
\]

That is, the solutions \(\Psi_2(t, x)\) and \(\Psi_3(t, x)\) do not satisfy a regular, time-independent, \(\gamma\)-Robin boundary condition at the boundary as \(\Psi_1(t, x)\) does.
We note that the analysis above could, in principle, be done for a massive field. However, closed forms expressions for the Fourier transforms in that case are not straightforward to obtain. Yet, the goal of illustrating the possible time-dependence feature of the generalized \((\gamma, v_k)\)-Robin boundary conditions is accomplished by the simplified, massless scenario above.

### 6.3 The Green functions

To construct the ground state for a Klein–Gordon field admitting generalized \((\gamma, v_k)\)-Robin boundary conditions on the two-dimensional half-Minkowski spacetime, we follow the rationale outlined in Sect. 5. On account of (25), the only unknown is \(\tilde{\psi}_2(x, x')\), which in turn can be constructed from the Green function \(\mathcal{G}(x, x')\) of the radial equation. Note that, in the case in hand, the rôle of the radial coordinate \(r\) is played by the cartesian coordinate \(x\). In addition, in this section, all values \(m_0 \geq 0\) are admissible.

Let the Wronskian between the principal and the secondary solutions be given by \(\{u, v_k\} = \Lambda_k\). Then the one between the two general square-integrable solutions given by (26) and (27) reads

\[
\{\psi_k(x), \psi_\infty(x)\} = \Lambda_k(b_k \cos(\gamma) - a_k \sin(\gamma)).
\]

Therefore, the Green functions \(\mathcal{G}_k(x, x')\) for the different choices of secondary solutions, which satisfy

\[
\left(\frac{d^2}{dx^2} + q^2\right) \mathcal{G}_k(x, x') = \left(\frac{d^2}{dx'^2} + q^2\right) \mathcal{G}_k(x, x') = \delta(x - x'),
\]

are given by

\[
\mathcal{G}_k(x, x') := \frac{\psi_k(x_<)\psi_\infty(x_>)}{\{\psi_k, \psi_\infty\}}, \quad \text{for} \quad q^2 \notin [0, \infty),
\]

where \((x_<, x_>\) = \((x, x')\) if \(x < x'\) and \((x_<, x_>\) = \((x', x)\), otherwise. Observe that the dependence on \(q\) is implicit in the solutions \(\psi_k\) and \(\psi_\infty\). Moreover, for \(\gamma \in \mathbb{R}\), it holds true that

\[
(b_k \cos(\gamma) - a_k \sin(\gamma)) = 0 \iff \cot(\gamma) = \frac{a_k}{b_k} \iff k = 1 \text{ and } \gamma \in \left(\frac{\pi}{2}, \pi\right).
\]

For notational convenience let us consider \(x < x'\) and \(\gamma \in [0, \frac{\pi}{2}]\) in the remainder of this section. Once more we fix \(s := \text{sign}(\text{Im}(q)), \text{Im}(q) \neq 0\). Explicitly, the Green functions can be written as

\[
\mathcal{G}_1(x, x') = -\frac{is}{2q} \left\{ e^{-isq(x-x')} + e^{isq(x+x')} \left[ 1 - \frac{2}{1 - isq \tan(\gamma)} \right] \right\},
\]

\[
\mathcal{G}_1(x, x') = -\frac{is}{2q} \left\{ e^{-isq(x-x')} + e^{isq(x+x')} \left[ 1 - \frac{2}{1 - is \tan(\gamma)} \right] \right\},
\]
$G_3(x, x') = \frac{-is}{2q} \left\{ e^{-isq(x-x')} + e^{isq(x+x')} \left[ 1 - \frac{2}{1 + is(1 + \cot(\gamma))} \right] \right\}.$

It is interesting to note that the three families of Green functions above share a translation-invariant part, but differentiate through a non-translation invariant remainder.

6.4 The resolution of the identity

For all three values of $\kappa$, the suitable contour to be considered for the integration of $G_\kappa$ is the “pac-man” in the $q^2$-complex plane, which is tantamount to integrating $2qG_\kappa$ in one semi-disk in the upper or lower $q$-complex plane, as illustrated in Fig. 1. Note that although $G_1$ and $G_3$ diverge in the limit $q \to 0$, $qG_\kappa$ has no poles in the $q$-complex plane. In addition, since Jordan’s lemma holds true, it follows that

$$-\frac{1}{2\pi i} \oint_{\text{“pac-man”}} G_\kappa(x, x') dq^2 = \lim_{R \to \infty} \int_{-R}^{R} q dq \lim_{\epsilon \to 0^+} [G_\kappa(x, x')|_{q+i\epsilon} - G_\kappa(x, x')|_{q-i\epsilon}] \quad (33)$$

Next, let us outline the computation of the integral given in (33), to highlight the fact that all three possible choices of a secondary solution does yield the resolution of the identity, as per (25). For $G_1$, this computation is standard, [24, Ex.7.3.2,Pg.454]. Yet, we do provide a step-by-step solution for all $\kappa$ in a supplementary notebook available online [25].

Observe that the common part of the integrand coming from the Green functions in (32) yields

$$-\frac{1}{2\pi i} \oint_{\text{“pac-man”}} \left\{ \frac{-is}{2q} \left[ e^{-isq(x-x')} + e^{isq(x+x')} \right] \right\} dq^2 = \delta(x - x') + \delta(x + x').$$
The remaining terms of $G_1$ and $G_3$ are obtained analogously to the above. For $G_1$, we use the Fourier transform
\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} dy e^{i\alpha y} \frac{1}{1 \pm iy} = e^{\mp \alpha} \Theta(\pm \alpha),
\]
and the extra term gives a vanishing contribution. Since both $x$ and $x'$ are positive, we obtain (25) for each $\kappa$:
\[
-\frac{1}{2\pi i} \oint_{\text{"pac-man"}} G_\kappa(x, x') dq^2 = \delta(x - x') + f_\kappa(\gamma) \delta(x + x') = \delta(x - x'),
\]
where we have introduced the auxiliary functions
\[
\begin{align*}
    f_1(\gamma) &= 1, \\
    f_2(\gamma) &= -\cos(2\gamma), \\
    f_3(\gamma) &= -\left[ \frac{2 \cos(\gamma)(2 \sin(\gamma) + \cos(\gamma))}{2 \sin(2\gamma) - \cos(2\gamma) + 3} \right].
\end{align*}
\]

With the spectral resolutions above, we can construct three one-parameter families of two-point functions, since it holds that
\[
-\frac{1}{2\pi i} \oint_{\text{"pac-man"}} G_\kappa(x, x') dq^2 = \int_{-\infty}^{\infty} dq \psi_\kappa(x) \psi_\kappa(x') \frac{\psi_\kappa(x) \psi_\kappa(x')}{N_\kappa},
\]
where the normalizations are given by
\[
\begin{align*}
    N_1 &= \pi q \left[ \cos^2(\gamma) + q^2 \sin^2(\gamma) \right], \\
    N_2 &= \pi q, \\
    N_3 &= \pi q \left[ 3 - \cos(2\gamma) + 2 \sin(2\gamma) \right] / 2.
\end{align*}
\]

### 6.5 The two-point functions

Directly from the spectral resolution, as stated in Sect. 5, we obtain the spatial part of the two-point function in each case:
\[
\tilde{\psi}_\kappa(x, x') = \frac{\psi_\kappa(x) \psi_\kappa(x')}{N_\kappa}.
\]

With the three choices of secondary solutions we obtain three one-parameter families of two-point functions for three different ground states in the 2-dimensional half-
Fig. 2 Behavior of $\mathcal{F} = \tilde{\psi}_\kappa(x, x')$ for $m_0 = 0.1, x = 1, \omega = -\Omega$ and $\gamma \in \{0, \pi/4, \pi/2\}$. On the left, for $\kappa = 1$. On the right, for $\kappa = 2$.

Minkowski spacetime:

$$\Psi_\kappa(t, x, t', x') = \int_0^\infty d\omega e^{-i\omega(t-t'-i0^+)} \Theta(\omega - m_0) \tilde{\psi}_\kappa(x, x').$$  (34)

We note that Eq. (34) only yields a well-defined distribution for $m_0 > 0$, due to the already mentioned infrared divergence.

**Remark 5** Figure 2 shows the behavior of $\tilde{\psi}_\kappa(x, x')$ at coinciding points $x = x' = 1$, for $\omega = -\Omega \in (m_0, 5)$, taking $m_0 = 0.1$, and for different values of $\gamma$. It manifests the inequivalence between the integrands of (34) for different values of $\kappa$. One may ponder on the significance of such discrepancy, since it could be the case that different integrands yield equal integrals (as it happens for the resolution of the identity, for example). Yet, as it turns out, the term $\tilde{\psi}_\kappa(x, x)$ has a physical interpretation: it characterizes the probability of de-excitations of a two-level system with energy gap $\Omega$, at a fixed spatial position $x$ and interacting for an infinite time with the quantum field in the ground state specified by $\Psi_\kappa(t, x, t', x')$. Such physical observable has been extensively used in the last years to probe a wide range of characteristics of the underlying quantum field theoretical framework, see [23, 26] and the references therein.

7 Conclusion

In this work we have highlighted the existence of a hidden freedom in the standard procedure of constructing ground states for a real scalar field in a large class of static backgrounds. In particular we have observed that, when working at the level of the radial equation, boundary conditions of Robin type can be imposed by using an arbitrary secondary solution. While this choice appears to be moot at the level of the underlying ordinary differential equation, it bears notable consequences at a fully covariant level. Interestingly, we have argued and shown via the concrete example of the two-dimensional half-Minkowski spacetime that, by exploring such freedom, one
can account for a large class of boundary conditions that are structurally quite different from regular Robin boundary conditions, possibly including time-dependent ones.

From a structural viewpoint, the choice of secondary solution does not alter the effectiveness of the methods used until now for the construction of ground on static spacetimes. Nevertheless, it does open the possibility of studying a much larger class of boundary conditions and of investigating the physical consequence of the various different choices. To conclude we emphasize that a rationale similar to the one considered in this paper can be taken also in the investigation of boundary condition of Wentzell type, see e.g. [18, 27]. Yet, a full-fledged analysis of this scenario would require a lengthy discussion that is worth leaving to a future work.

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