Semi-classical aspects of black hole formation and evaporation

Towards a rigorous understanding of black hole space-times as solutions to the semi-classical Einstein equations

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Referat

Eine Untersuchung offener Probleme zur Verdampfung schwarzer Löcher im semi-klassischen Modell, bezüglich der Existenz von Quantenfeldtheorien auf Raumzeiten, die verdampfende schwarze Löcher beschreiben, sowie der Existenz von Lösungen der semi-klassischen Einstein Gleichungen, welche schwarze Löcher darstellen.

An investigation into open problems related to black hole evaporation in the semi-classical framework, concerning the existence of quantum field theories on spacetimes modelling evaporating black holes as well as the existence of black hole solutions to the semi-classical Einstein equations.

Abstract

Approximately 50 years ago it was predicted that black holes, once formed, leak away their mass via Hawking radiation, such that they either shrink to a very small size or completely disappear. This idea gave rise to a long-standing debate, as this shrinking, or colloquially evaporation, of black holes seems to lead to non-unitary time evolution of quantum field theories defined on these background geometries. For many, this is an unappealing feature. Hence it is often argued that some fundamental phenomenon beyond the semi-classical regime should intervene in the evaporation process and restore unitarity of time evolution. Unfortunately, even on a semi-classical level, black hole evaporation is far from fully understood. It is not known if there are any solutions to the semi-classical Einstein equations, which can be used to characterize semi-classical gravity, that describe formation and evaporation of black holes. Nor is it fully clear where semi-classical gravity gives a reasonable description of actual physics. In this dissertation we discuss some open problems concerning semi-classical gravity in relation to black hole spacetimes. In particular, we present an investigation into the compatibility of spacetimes describing full black hole evaporation (and other spacetimes with a similar causal structure) and algebraic quantum field theory. Secondly, we present an approach that allows for the formulation of the semi-classical Einstein equations as a (characteristic) initial value problem, which can be used as a starting ground into the investigation of black hole solutions.

This dissertation is a cumulative work, consisting of two publications. The first publication introduces a class of spacetimes, namely semi-globally hyperbolic spacetimes, which generalize certain features of fully evaporating black hole spacetimes. Spacetimes like these may be used to model the low-curvature regime of a full black hole evaporation spacetime, where semi-classical gravity (or some more detailed effective field theory of gravity) is expected to be valid. In order to investigate the feasibility of such a point of view, the existence of quantum field theories is investigated on these backgrounds. It is found that while algebras of observables on these spacetimes are straightforward to construct, the existence of globally defined sensible quantum states depends in a non-trivial way on the geometry of a black hole evaporation spacetime near its singularity as well as the regime where one wishes semi-classical gravity to be implemented.

The second publication focusses on the semi-classical Einstein equations, which couple a classical background geometry to a linear scalar quantum field propagating through it. Following recent investigations into cosmological solutions of these equations, we wish to formulate an initial value problem for spherically symmetric solutions, which are hoped to contain black hole solutions. Rather than formulating a Cauchy problem, with initial data given on some space-like Cauchy surface, we argue that in this context it is more convenient to formulate a Goursat problem, with initial data given on some characteristic cone. We derive a constraint reminiscent of the Hadamard condition on initial quantum states defined on these cones that guarantee observables relevant to semi-classical gravity to admit finite expectation values at the initial surface, and we derive an expression for these values. Furthermore, we show how this formalism can be used to explicitly calculate expectation values of these observables in the domain of the dependence of the null cone from some initial quantum state, both as a linearised expression and as a formal perturbation series in some parameter appearing in the metric.

Keywords

Quantum Field Theory on Curved Space-times, Semi-classical Gravity, Black Hole Evaporation, Non-globally Hyperbolic Space-times, Hadamard States, Goursat Problem

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Preamble

1. Introduction

It is perhaps fair to say that one of the most influential results from quantum field theory on curved background spacetimes is that, when a quantum field propagates on an (astrophysical) black hole spacetime, an observer at infinity will eventually observe the field configuration to be that of thermal radiation coming from the direction of the black hole. First predicted in Ref. [1], it has become known as the *Hawking effect*, or *Hawking radiation*. Even though any experimental probing of this effect is still out of reach,[1] the potential ramifications of this effect have had a major impact on the further development of theoretical physics, of course within the field of quantum field theory on curved spacetimes itself, but certainly also on quantum gravity.

Two ramifications stand out, one being that, through the temperature associated with Hawking radiation, a black hole could be assigned a finite temperature. For a Schwarzschild black hole of mass M, this *Hawking temperature* can be found to be (in Planck units)

$$T_H = \frac{1}{8\pi M}. \tag{1.1}$$

This corroborates a previously noted analogy between the dynamics of black holes and the laws of thermodynamics (see Ref. [4]). It is a still unsettled debate as to what degree this analogy is more than mathematical, and in particular to what extent the similarities between the macroscopic laws of black hole dynamics and thermodynamics imply that black hole physics derives from a statistical treatment of microphysics. Most noteably, can black hole entropy due to Bekenstein and Hawking,

$$S_{BH} = \frac{A}{4}, \tag{1.2}$$

[1]That is to say, while experimental observations of Hawking radiation produced by actual black holes is certainly not yet feasible, theoretically analogous effects have been observed in more 'table-top' size systems that share some similarities with black holes as predicted by General Relativity, see e.g. Ref. [2, 3]. Though these systems may present an interesting testing ground for certain aspects of Hawking radiation, in the absence of any experimental proof that the analogy between these systems and actual black holes occurring in nature is sufficiently strong, it is difficult to conclude anything definitive from these experiments about the Hawking effect as it pertains to astrophysical black holes.

with A the area of a Schwarzschild event horizon, be interpreted as a statistical measure for the number of microstates available to describe the macroscopic system à la Boltzmann. Calculations from various approaches towards quantum gravity certainly suggest such an interpretation is possible, see e.g. Ref. [5] based on a string theory model (see also Ref. [6] for a conceptual review of this influential calculation), and Ref. [7] for a similar result from loop quantum gravity. However, there does not seem to be any widespread consensus what degrees of freedom actually ought to contribute to this entropy measure: Those describing the near horizon region, or those describing the full black hole (see Ref. [8]).

Hawking's original paper inspired a thorough investigation into the thermal properties of quantum field theories on spacetimes with horizons. This lead to the discovery of the *Unruh effect* (Ref. [9]), and the observation that both these effects relate to the *Bisognano-Wichmann theorem* (Ref. [10]), which the thermal nature of the Minkowski vacuum state (restricted to some wedge region) with respect to the flow of Lorentz boosts (see Ref. [11, 12]). Furthermore, a general theorem showing the thermal nature of stationary, and sufficiently regular (i.e. Hadamard), quantum states on spacetimes with an (asymptotically time-like) Killing field and bifurcate Killing horizon is proven in Ref. [13]). Though these discoveries should not be understood as equivalent to the Hawking effect,[2] the relation between the presence of Hawking radiation and the thermality of stationary Hadamard states near horizons can certainly be made precise, as done in Ref. [14]. Broadly speaking, due to gravitational redshift of signals coming from a neighbourhood near a black hole horizon that reach asymptotic infinity, an observer receiving such signals, in this case propagated by a quantum field, is probing the short distance behaviour of the state of that field near the horizon (i.e. its scaling limit). For a given (linear scalar) quantum field, such a scaling limit at a point in a spacetime is universal for any Hadamard state near that point, and hence at a horizon is identical to that of a thermal equilibrium state. Thus the signals received by the asymptotic observer from this region closely resemble those given off by a thermalized body, particularly one at the Hawking temperature. These signals, which in this case are simply the n-point functions of the quantum state as they propagate through the spacetime, are what is observed as Hawking radiation. Such a scaling limit can in fact be shown to have thermal properties for a much wider class of (dynamical) horizons than a Killing horizon (see Ref. [15]). In studying the correlations between the quantum states defined on these scaling limit theories, one can

[2] After all, the spacetime associated with a black hole formed by gravitational collapse is certainly not stationary.

use the notion of relative entropy to arrive at an entropy concept for a black hole horizon that behaves precisely as the Bekenstein-Hawking entropy, in so far that it scales with the area of the horizon. This supports the view that a microscopic interpretation of the laws of black hole dynamics may not necessarily require a framework of quantum gravity, but can be fully stated in terms of quantum field theory on curved spacetimes. To some extent, this has some conceptual advantages, as in this scenario all thermodynamic quantities at play, in particular the temperature and the entropy of the horizon, can be given a microscopic definition in the same framework, while quantum-gravity-based approaches focus mainly on the latter quantity. However, it is less clear how, if at all, one could hope to derive the macroscopic laws of black hole dynamics from these microscopic interpretations, as they do not in themselves relate directly to geometric degrees of freedom and their dynamics. Still, at the Planck scale, geometric and matter degrees of freedom may not be so easily distinguished, or at least will be correlated. Thus, it may well be that the scaling limit entropy considered in Ref. [15] can be seen as some semi-classical limit of a more fundamental entropy concept.

The second ramification of the Hawking effect, and the one more relevant to the articles that make up this dissertation, is the fact that, in principle independently of the thermal nature of Hawking radiation, it carries away energy from the neighbourhood of a black hole towards asymptotic infinity. More precisely, one can calculate an outgoing positive energy flux at asymptotic infinity associated with Hawking radiation (see again Ref. [1]). Under some general assumptions, in particular stress-energy conservation and approximate stationarity of the late-time quantum state, this implies that through the black hole horizon one should have an energy flux of opposite sign, i.e. some radiation carrying negative energy into the black hole. Already at a heuristic level, this would imply that through this process the mass of the black hole decreases and hence that the black hole shrinks.[3] This process is generally referred to as *black hole evaporation* and even though for any macroscopic black hole this process of evaporation would be practically immeasurably slow, the theoretical possibility of a black hole shrinking to an arbitrarily small size through a radiative process that is (apart from the total mass, angular momentum and charge) insensitive to whatever is inside the black hole, has confounded many physicists in the years following the prediction of this process. Particularly the fact that through this process a black hole may

[3]That the somewhat heuristic picture above of the outgoing energy flux at infinity implying a decrease of the area of the black hole horizon is not trivial to make precise, and requires some non-obvious assumptions, is illustrated in Ref. [16].

eventually fully "evaporate", and that this may not only apply to macroscopic (say of Solar mass and heavier) black holes, but also to microscopic black holes (either primordial or possibly those playing a role in quantum gravity processes, for instance akin to virtual particles in more familiar scattering processes of quantum fields, or those contributing in a 'sum over histories' approach to quantum gravity), suggest a fundamental irreversibility, or at least breakdown of unitary time-evolution in quantum gravity (see Ref. [17, 18]).

This last observation, and its clash with the foundations of the most popular approaches to quantum gravity (and the intuition of many major figures in these fields), has come to be known as the 'information loss paradox' (see Ref. [19]).[4] Hawking radiation and black hole evaporation are semi-classical concepts, but it is a valid question what would happen to these processes if quantum effects of gravity (whatever they may be) are properly taken into account. Guided by the assumption that a theory of quantum gravity should indeed be unitary, in the sense that the time evolution of the theory bijectively maps pure states to pure states (see Ref. [21]), many have aimed to identify a mechanism beyond semi-classical physics through which unitarity is restored, often motivated by various toy models in quantum gravity. Here I shall not attempt to give an exhaustive list of these proposed mechanisms. Some listings of (at some time) popular proposals can be found in the references [19, 22]. I merely shall distinguish two classes of proposals, those that agree with the conjectured semi-classical black hole evaporation apart from deviations in some (microscopic) 'high curvature regime', which, see e.g. Ref. [23], are sometimes referred to as *conservative* approaches, and proposals that deviate from semi-classical (or effective field theory) physics on macroscopic scales, called (perhaps somewhat abusively) *radical* approaches. Examples of conservative approaches are certain remnant scenarios (see e.g. Ref. [24]) or black-hole-to-white-hole transition scenarios (Ref. [25]), while among the radical approaches one can count black hole complementarity (Ref. [26]) and fuzzballs (Ref. [27]). With conservative resolutions readily available, one may wonder why these radical approaches are so seriously considered. One of the main reasons that some deem a radical resolution necessary, is the so-called *Page curve* argument made in Ref. [28], which entails that if the end state of black hole evaporation is to be pure (given a pure initial state), the 'release' of information from the black hole should take place over macroscopic time-scales. This argument is however based on rather strong assumptions about the statistical origin of black hole thermodynamics. As

[4]In a personal account of an influential participant in the discussion surrounding the paradox (Ref. [20]), this clash has even been framed as 'the Black Hole War'.

discussed, this is a debated issue.

The state of affairs is thus a zoo of proposals, both conservative and radical, aimed at ensuring unitarity of black hole evaporation, which all have their pros and cons both based on general requirements as well as assumptions tied to particular theoretical frameworks used to understand the microphysics of spacetime and gravity. It is often difficult to fully penetrate the assumptions that underlie a particular proposal and without a way to establish a 'correct' theory of quantum gravity, it will remain unclear which of these proposals, if any, is correct. This is not helped by the fact that, even in the semi-classical framework from which the concept of black hole evaporation originates, this process is not fully understood. It is hence worthwhile to take a step back and address some important open questions: To what extent is this process consistent within the semi-classical framework itself, can one rigorously show that black hole evaporation occurs in semi-classical gravity and if so, what can one expect to be the range of validity of such a black hole evaporation solution? This dissertation shall explore concepts with which these questions may be better understood, so as to put the information loss debate on firmer foundations.

1.1 The semi-classical Einstein equations

For the purposes of this work, semi-classical gravity is taken to be characterized by a (linear, scalar) quantum field defined on a class of classical curved background spacetimes, where the background geometry (M, g) and the state ω of the quantum field are such that the semi-classical Einstein equations are satisfied, i.e.

$$G_{\mu\nu} = \kappa\langle : T_{\mu\nu} : \rangle_\omega, \tag{1.3}$$

where $G_{\mu\nu}$ is the Einstein tensor associated with the metric g, $\langle : T_{\mu\nu} : \rangle_\omega$ is the expectation value of a locally covariantly renormalized stress energy tensor of the quantum field theory evaluated in the state ω (usually taken to be Hadamard such that $\langle : T_{\mu\nu} : \rangle_\omega$ is surely finite) and κ a coupling constant associated with the Newton constant. For the precise notion of a linear scalar quantum field and the renormalized stress-energy tensor, the reader is pointed to the attached publications and references therein. See in particular Sec. 2.3 and 4 of Publication II.

The semi-classical Einstein equations (abbreviated s.c.E.eqs.) are viewed as a natural generalization of the classical Einstein equations to the context of quantum field theory and one hopes that solutions to this equation in some sense approximate a solution within a full theory of quantum gravity in certain regimes. However, in the absence of a full theory, only formal arguments for such a statement are available, see e.g. Ref. [29] where some of these arguments are collected. In this context, the metric g (or rather, the geometry described by the diffeomorphism class of (M, g)) is interpreted as an expectation value of a 'quantum' metric subject to quantum fluctuations. However, as diffeomorphism classes of Lorentzian geometries do not form a convex space under any obvious notion of convex sums, it is a priori not clear if such an expectation value can be defined consistently. Hence, one usually only expects such an interpretation to be sensible if the fluctuations in the geometry are, in some appropriate sense, small. If one accepts this assumption, typical justifications of the use of the semi-classical Einstein equations furthermore depend on the further assumption that any quantum effects due to present matter fields dominate those of pure gravity contributions. For instance, in an approach where the s.c.E.eqs. are derived using perturbative methods around some vacuum solution to classical Einstein equations, the semi-classical Einstein equations hold at first loop order (or formally at first order in $\hbar$) under the assumption that one-loop pure graviton contributions can be ignored (see Ref. [30, 29]). More generally, one may view the classical scalar field as a place-holder for purely gravitational effects, assuming that one-loop contributions of gravitons behave qualitatively similar to scalar fields. In this latter point of view, the semi-classical Einstein equations are, in some sense, a toy model for effective quantum gravity. Alternatively, if instead of considering a single quantum field, a large number of fields are assumed to contribute to the total stress-energy tensor, these contributions will automatically dominate quantum gravitational effects in any low curvature regime and as a result the s.c.E.eqs. formally follow (see Ref. [31]).

Early investigations into the semi-classical Einstein equations mostly focused on the linearised equations around Minkowski spacetime, mostly based on an axiomatic approach to a calculation of the stress-tensor (see Ref. [32]). This linearised model clearly reveals some pathologies associated to the semi-classical Einstein equations. First of all, due to the way the metric enters into the renormalization of $\langle : T_{\mu\nu} : \rangle_\omega$,[5] the (linearised) s.c.E.eqs. coupled to some linear scalar field contain up to fourth order derivatives of the metric and in particular, in coordinates adapted to a standard 3+1 split, contain up to fourth order time-derivatives. Due to this, fixing a solution to these equations will typically require more initial data then what is required for the Einstein equations coupled to a classical scalar field. For an initial value problem on some space-like Cauchy surface, one would expect to require at least up to

[5]The renormalization scheme is assumed to satisfy the requirements detailed Ref. [33, Sec. 4.6], and is in particular locally covariant (see Ref. [34, 35]).

third order time-derivatives of the metric at this surface as geometric input, which (ignoring constraints) effectively doubles the size of the phase space associated with the spacetime geometry in comparison with the classical Einstein equations. Moreover, already at this linearised level, solutions to these equations are unstable, as many solutions to the linearised equations show runaway behaviour, such that small perturbations of the metric can grow exponentially in some time-parameter. These runaway solutions therefore quickly leave the regime in which at the very least the linearised equations, but in principle also the full semi-classical Einstein equations, may be expected to hold. Moreover, such instabilities (in particular of Minkowski spacetime) are not observed in nature. Therefore this runaway behaviour is typically deemed nonphysical.

Several methods have been proposed to remove this nonphysical behaviour from the class of solutions to the semi-classical Einstein equations, and give selection criteria on which solutions should be deemed as physical. One such proposal is to only consider solutions that can be seen as corrections to solutions to the classical Einstein equations, where the full semi-classical solution is analytic in $\hbar$ (see Ref. [36]). Finding such solutions to the s.c.E.eqs. then involves solving a second order differential equation for each order in $\hbar$. This can be seen as an order reduction scheme to the semi-classical equations. A similar order reduction scheme has been applied to the linearised s.c.E.eqs. in Ref. [29], in order to study solutions to this equation to order $\hbar^2$.

For these solutions, it is shown in Ref. [29] that, in the regime where the order-reduced linearised Einstein equations can be assumed to be valid (and under some further assumptions concerning spacetime geometry at past asymptotic infinity), the stress-energy tensor appearing on the right hand side of the order-reduced equation satisfies a nontrivial energy condition, namely a transversely smeared averaged null energy condition. As reviewed in [37], energy conditions of this type, i.e. particular restrictions on certain components of the stress-energy tensor on a given class of spacetimes, are instrumental in proving singularity theorems. In the context of black hole evaporation, one can wonder if gravitational collapse in semi-classical gravity lead to the formation of a singularity (or more concretely, whether a Penrose-type singularity theorem holds in this context), or if, through semi-classical effects, the interior geometry of the black hole is regularized. At this point in time, no Penrose-type singularity theorem has been formulated using an energy condition that has been rigorously shown to hold for quantum fields on curved backgrounds relevant to four-dimensional black hole formation and evaporation.

The last decade saw developments in the study of solutions to the full semi-classical Einstein equations. These are discussed in the next section.

1.1.1 Known solution classes

Solutions to the full semi-classical Einstein equations have been studied particularly in the context of cosmological models, see e.g. Ref. [38, 39, 40, 41, 42]. More specifically, these works study solutions to the s.c.E.eqs. where the spacetime takes the form of a 3+1 dimensional spatially flat Friedman–Lemaître–Robertson–Walker spacetime $\mathbb{R} \times \mathbb{R}^3$ with metric

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a(t)^2 \gamma_{\mathbb{R}^3} \tag{1.4}$$

where $\gamma_{\mathbb{R}^3}$ is the standard Euclidean metric on $\mathbb{R}^3$, and where the linear scalar quantum field is assumed to obey the equation of motion

$$(\Box - m^2 - \xi \mathfrak{R})\phi = 0, \tag{1.5}$$

with $\Box$ the Laplace-Beltrami operator, m a mass, ξ a dimensionless coupling and $\mathfrak{R}$ the Ricci scalar. Furthermore, it is assumed that the field is in a 'sufficiently regular' quasi-free state ω of which the two-point function is homogeneous and isotropic.[6] Due to the symmetries of the spacetime and the quantum state, it is convenient to expand the spatial dependence of the two-point function in Fourier modes. As shown in [39], one can implement a locally covariant renormalization scheme directly onto these Fourier space two-point functions, such that one can rewrite the semi-classical Einstein equations (or in particular their trace) in relatively tractable form.[7] This formulation of the s.c.E.eqs. forms the basis for their analysis as an initial value problem in [38, 40, 42]. Further relying on the previously mentioned Fourier decomposition of two-point functions, constraints on initial data for the quantum state can be formulated such that it is sufficiently regular for the relevant renormalized quantities to admit finite expectation values. Furthermore, as worked out in detail in [42], it turns out to be convenient to introduce an auxiliary reference state (the construction of which relies on some further geometric assumptions) which can be used to isolate the contributions to the s.c.E.eqs. that are associated with the pathologies previously discussed for the linearised equations. This allows one to rewrite the semi-classical equations in a form for which local existence of solutions (i.e. on some finite time interval) subject to some

[6] Sufficiently regular is made precise in Ref. [42], and comes down to a generalized Hadamard condition.

[7] For the case of conformal coupling, i.e. $\xi = \frac{1}{6}$, a similar result had also been derived in [38].

particular initial data can be shown by formulating it as a fixed point problem.[8]

A second approach to studying exact cosmological solutions, carried out in Ref. [43], has been to classify static solutions, in this case those where the geometry takes the form of a (spatially compact) Einstein's static universe $\mathbb{R} \times S^3$ with metric

$$ds^2 - \mathrm{d}t^2 + a^2 \gamma_{S^3}, \tag{1.6}$$

for γ_{S^3} the metric of the unit three-sphere (as embedded in the Euclidean $\mathbb{R}^4$). Similarly to the case above, one can expand sufficiently symmetric two-point functions in terms of well-understood functions that are suitable to the symmetry of the problem. Under some geometric assumptions, one also can introduce a reference state on these geometries, in this case the ground state of the quantum field theory. The semi-classical Einstein equations can now be formulated fully in terms of the expansion coefficients associated with a (sufficiently regular) two-point function and geometrical quantities, which can be used to prove a variety of results for states and geometries solving these equations.

As noted, the methods alluded to above make convenient use of the symmetries of both the spacetime and the two-point functions under consideration. Expanding a two-point functions into decoupled contributions, such as into Fourier modes as in the analysis of [42], naturally loses much of its power once one considers spacetimes of lower symmetry. Especially in a setting of a dynamical spacetime, one can argue that a mode-expansion-based treatment of quantum fields is not necessarily the most natural.[9] In order to extend our understanding of exact solutions to the semi-classical Einstein equations to a more general class of spacetimes, such as those describing black hole formation and evaporation, it may be useful to develop further techniques for analysing the evolution of states on a quantum fields and their associated expectation value of the stress-energy tensor without deferring to such expansions. This is the main motivation of Publication II.

[8] Extending this local existence result a global result has so far only been carried out for conformal coupling $\xi = \frac{1}{6}$, see [40].

[9] Nevertheless, even in the case of very little symmetry, mode expansion techniques may still prove useful in some contexts, particularly in the case of spacetimes with asymptotic symmetries, where mode decompositions prove useful in defining initial states, or in some numerical approaches see e.g. Ref. [44, 45].

1.2 Some open problems for semi-classical black hole evaporation

As discussed briefly in the introduction, the prediction of the Hawking effect naturally leads to the conclusion that black holes can shrink in size (i.e. evaporate) over time due to the fact that their energy is radiated away via Hawking radiation. For black holes significantly larger than the Planck mass this should be a very slow process, simply due to the fact that the Hawking radiation has a comparatively tiny temperature for large black holes.[10] Nevertheless, one expects that after a long period of time a black hole may eventually shrink to Planck size (in the sense that local curvature scalars near the apparent horizon approach 1 in Planck units),[11] where one cannot reasonably expect any classical geometry to accurately describe the near-horizon physics. Still, in the absence of any clear mechanism that would slow down the production of Hawking radiation as the black hole shrinks, it is a priori not unreasonable to assume that even a Planck-size black hole would continue to lose energy until it completely disappears. Therefore, in Ref. [1], Hawking posits that a spacetime describing the complete lifetime of a black hole, detailing both its formation and evaporation, should have a Penrose diagram similar to Fig. 1.1.

In principle, this Penrose diagram should be taken with some grains of salt. It describes a spacetime with a naked singularity, in the sense that the spacetime contains inextendible causal curves that are completely contained in the domain of outer communication $I^-(\mathscr{I}^+) \cap I^+(\mathscr{I}^-)$, which is associated with a Planckian curvature regime (i.e. the evaporation of the Planck-size black hole). Therefore, one should only think of Fig. 1.1 as an effective description of a hypothetical full evaporation process, where the local physics away from the Planckian regime can be treated via semi-classical gravity or effective quantum gravity, while input from a full quantum gravity theory may be required to give a consistent description of the physics in the high-curvature regime. In order to investigate if this point of view can be made precise, and to understand what kind input from Planck scale physics would be required to consistently define such an effective description of black hole evaporation, one requires a framework to treat quantum field theories on geometries such as a

[10] Even though usual calculations of the Hawking effect are performed on stationary backgrounds, or at least stationary post some gravitational collapse process (see also Ref. [46, 14]), results from these calculations are thought to still be applicable in a quasi-stationary regime where black holes shrink only very slowly.

[11] This assumes that during the evaporation process, no further matter will fall into the black hole, as this would again increase its size. However, to prevent a black hole from shrinking, such a matter influx would have to be quite fine-tuned.

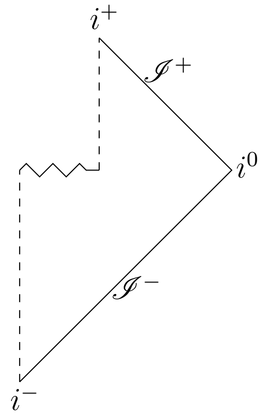

Figure 1.1: A Penrose diagram of an evaporating black hole as drawn in Ref. [1]

black hole evaporation spacetime or, in an appropriate sense, approximations thereof. Such a framework is provided in Publication I.

As discussed in Publication I, the presence of the naked singularity, sometimes referred to as the 'evaporation event', means that a (classical) spacetime describing a fully evaporating black hole cannot be globally hyperbolic, or even causally continuous (see Ref. [47]). In fact, one can view the breakdown of global hyperbolicity due to full black hole evaporation as the main cause of information loss. Any notion of global time evolution for quantum field theory on some background spacetime can only be expected to be unitary if it is defined with respect to a global notion of time for which the equal time slices are Cauchy surfaces,[12] which in particular requires the background spacetime to be globally hyperbolic (see e.g. Ref. [21]). From a purely quantum field theory perspective, information loss in itself is therefore not a problematic aspect. However, if the spacetime in question is not globally hyperbolic, then standard constructions of (linear scalar) quantum field theories such as in Ref. [49], or results on global existence of well-behaved quantum states (such as Ref. [50]) are not generally applicable.

Similar problems (or features, if you will) are known to occur for a variety of non-globally hyperbolic spacetimes that appear in other contexts. A prime example of this is given in Ref. [51], concerning spacetimes with 'compactly generated Cauchy horizons' (which relate to models of universes in which a 'time machine' has been manufactured). Here it is shown that

[12] This is a property that in the context of algebraic quantum field theory is formulated in terms of the time slice axiom, see e.g. Ref. [48].

a linear scalar quantum field theory defined on some globally hyperbolic sub-spacetime cannot be extended to the full spacetime in a sensible manner (i.e. as an 'F-local' quantum field theory, see Ref. [52] or Publication I). A related result is derived at the level of two-point functions, namely that any extension of a well-behaved (i.e. Hadamard) two-point function on this sub-spacetime to a globally defined two-point function (i.e. a bi-distribution satisfying the equation of motion) cannot be locally Hadamard at every point (in the sense of Ref. [13]), which concretely means that non-linear observables such as Wick squares $:\Phi^2:$ or the stress-energy tensor $:T_{\mu\nu}:$ may not be defined everywhere. More recently, inextendibility of Hadamard two-point functions has been observed for certain black hole spacetimes with non-globally hyperbolic interior in Ref. [53, 54], where in particular components of the stress-energy tensor have been shown to diverge near Cauchy horizons on certain Reissner-Nordström-deSitter black holes.

An example of such an inextendibility result of Hadamard states that, in light of Publication I, has some relevance to the black hole evaporation spacetime, has been found in Ref. [55]. Here a quantum field theory is considered on a so-called trouser spacetime, a 1+1-dimensional flat geometry that undergoes a topology change.[13] The causal structure of these topology-changing geometries and the causal structure given by Fig. 1.1 can be seen as similar, in a sense made precise in Publication I, namely that these geometries are *semi-globally hyperbolic*. However, as the naked singularity of black hole evaporation spacetimes is not merely topological, but rather a curvature singularity, generalizations of these types of arguments to the setting of black hole evaporation are unfortunately not available.

With the examples above in mind, one cannot reasonably assume that a quantum field theory on a full black hole evaporation spacetime admits any globally defined well-behaved quantum states. This further indicates the need for Planck-scale physics to be properly accounted for in at least a finite-size high-curvature regime of the evaporation process, not just to give a physically accurate description of black hole evaporation, but rather to give a mathematically consistent one. Such mixed models of (semi-)classical physics in a low-curvature regime and input from quantum gravity near the high-

[13]Ref. [55] focuses on a massless theory, and presents an argument involving an initial vacuum state (modulo the divergent zero-frequency mode contributions) which can be extended to the full spacetime, but fails to yield a finite energy density expectation value on the Cauchy horizon induced by the topology change. Using ideas from Publication I and the results on local quasi-equivalence of quasi-free Hadamard states and Ref. [56, Prop. 3.5], these results can be generalized to extending arbitrary Hadamard states for both massless and massive theories on this trouser spacetime, as well as for some higher dimensional geometries.

curvature regime have for instance been considered in a somewhat qualitative sense in Ref. [25], where some of these models even seem to predict observable consequences (see e.g. Ref. [57]). The framework of Publication I may be used to treat the low-curvature regime (both pre and post evaporation) in these types of models.

For a full dynamical treatment of the semi-classical regime of black hole formation and evaporation that goes beyond the heuristic arguments already put forward in Ref. [1], one would like to study black hole solutions to the semi-classical Einstein equations. Unfortunately, it is not known if such solutions even exist, let alone what they look like. In fact, this has been a major open problem that has frustrated the discussion on black hole evaporation for the past four decades. This is partly because for a quantum field on a general spacetime background, it is very difficult to explicitly calculate the expectation value of the stress energy tensor in any given state. Consider for example the Unruh state on a Schwarzschild spacetime, which is used to model Hawking radiation at significant distance from a collapsing body forming a (classical) black hole. Only by numerical methods developed in the last decade could the stress-energy tensor be evaluated at any finite distance from the black hole (see Ref. [45]). While in principle these methods can be generalized to more dynamical situations (see e.g. Ref. [58]), one quickly runs into practical limitations of numerical analysis when trying to perform these calculations.

Although the Unruh state evaluations may give some useful insights into a solution to the backreaction problem, i.e. taking the effects of Hawking radiation into account when evolving the semi-classical Einstein equations, one typically only expects this Unruh state to give a reasonable approximation to the stress-energy tensor appearing in this full problem when one restricts oneself to some adiabatic regime. It has been put forward on numerous occasions that semi-classical effects may have a significant impact on the way black holes, or more specifically trapped surfaces, form during gravitational collapse, see e.g. Ref. [59, 60, 61].[14] Such processes would take place in a regime that is certainly not adiabatic, but could definitely alter the original picture of black hole evaporation sketched in Fig. 1.1. This highlights that gaining a better and more rigorous understanding of both semi-classical black hole formation and evaporation is, although a major challenge, certainly worthwhile to attempt. Taking inspiration from developments concerning the

[14]Some of these proposals appear to have some non-physical implications, see e.g. Ref. [62], however these objections focus on the most simplified models for these collapse mechanisms.

semi-classical gravity in the cosmological setting, which was shortly discussed in the previous section, Publication II aims to develop an approach with which (existence of) spherically symmetric solutions to the s.c.E.eqs. may be studied, which might in particular be used to analyse solutions describing gravitational collapse.

Publication II takes inspiration from references [38, 39, 40, 41, 42] , which concern themselves with the cosmological setting, in the sense that it aims to provide a set-up in which the semi-classical Einstein equations (under assumptions of spherical symmetry) can be studied from the perspective of an initial value problem. In what it achieves, Publication II is most closely analogous to Refs. [38, 39]. Similarly to what had been undertaken in these references for FLRW spacetimes, Publication II provides a globally defined regularization scheme for (Hadamard) correlation functions (of some linear scalar quantum field theory) defined on observables localized on some partial Cauchy surface (in the sense of Ref. [63]). This allows the s.c.E.eqs. to be formulated in terms of geometric data at these surfaces and this regularized two-point function. Nevertheless, the approach advocated in Publication II and the approach used in the cosmological setting also differ on a number of key points. Firstly, the correlation functions in Publication II are represented in position space, using some particular parametrization of the partial Cauchy surfaces on which they are defined, rather than via a Fourier-space representations such as is available on the highly-symmetric FLRW spacetimes. Secondly, instead of considering correlation functions over space-like full Cauchy surfaces (such as the slices of equal cosmological time for FLRW backgrounds), the partial Cauchy surfaces considered in Pub. II are characteristic surfaces, namely surfaces ruled by null geodesics emanating from a point on the axis of spherical symmetry. This also means that the type of initial value problem for which the results of Pub. II can be used, is a characteristic initial value problem (or Goursat problem) rather than a Cauchy initial value problem. In contrast, a Cauchy initial value problem approach to the full s.c.E.eqs. has recently been investigated in Ref. [64]. This work highlights the subtleties involved in setting up initial data that define a Hadamard state on the full spacetime. As illustrated in Pub. II, relying in part on the results of Ref. [65], these issues are less problematic when initial states are defined on a characteristic surface, at least under the assumption of spherical symmetry. Note furthermore that for classical scalar fields, a characteristic approach to the Einstein equations has proven useful in the past to study gravitational collapse and black hole formation, see Ref. [66, 67].

As noted above, Pub. II introduces a global regularization scheme for

Hadamard correlation functions restricted to a lightcone surface. It achieves this through constructing a Hadamard parametrix that is globally defined on these characteristic surfaces, which is in contrast to the usual construction of (locally covariant) Hadamard parametrices (see e.g. Ref. [13]), as the latter construction typically only yields a parametrix on geodesically normal neighbourhoods. Directly extending this construction to yield a Hadamard parametrix on, say, some neighbourhood of a (partial) Cauchy surface is in principle possible, see e.g. Ref. [68], but in general a far from straightforward or tractable procedure. The construction of the *characteristic* Hadamard parametrix defined in Pub. II circumvents these difficulties by making explicit use of the lightcone geometry, which makes it a quasi-local (and arguably quite manageable) procedure. The resulting regularized characteristic two-point functions (yielded from subtracting the characteristic Hadamard parametrix from Hadamard two-point functions on some lightcone) are shown to satisfy a dynamical equation, which can be used to gain global control on expectation values of renormalized observables. Using this 'equation of motion' for the regularized two-point functions, one can in principle calculate (or at least approximate) the expectation values of non-linear observables in the causal future of the characteristic surface on which some initial state has been defined. In Pub. II this is illustrated by a linear-order calculation (in terms of deviations of the background metric from a Minkowski background) of $\langle :\Phi^2: \rangle$ for a massless field on a Vaidya spacetime evaluated in the past asymptotic vacuum state, but this method can certainly also be applied to calculate linear-order contributions to the stress-energy tensor, which can be shown to match the results of Ref. [32]. At a formal level, one can give an expression to arbitrary order in metric perturbations, though in practice these will still be challenging to calculate. Nevertheless, one can certainly use the results of Pub. II to go beyond linear-order calculations, as using techniques from Ref. [69], global estimates on expressions involving the regularized two-point function (and in particular on certain coincidence limits) can be derived. These estimates are not yet presented in Publication II. Nevertheless, these ideas point towards a promising direction for further applications of the results presented in this dissertation, in particular in the context of studying the solutions to the s.c.E.eqs., where such estimates may play an important role.

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Publications

I. Quantum fields on semi-globally hyperbolic space-times

Outline

Content

Bibliographic Information

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Summary of Publication

In light of recent discussions on the causal structure of a black hole evaporation spacetime and its impact on quantum field theories on these backgrounds, as discussed for instance in [1, 2, 3], this work introduces a class of spacetimes with causal structure sharing some particular aspects with the Penrose diagram that is usually associated with an evaporating black hole. These spacetimes, dubbed semi-globally hyperbolic spacetimes, can, loosely speaking, be seen as globally hyperbolic up to some causal defects located on a discrete set of time-slices. This class can be characterized in a variety of equivalent ways, most notably via the existence of a global time function with particular properties or via a covering by globally hyperbolic sub-spacetimes.

Using the latter characterization, a notion of a quantum field theory can be introduced on these spacetimes which relies on a strengthened version of F-locality, i.e. a minimal requirement for quantum field theories on arbitrary non-globally hyperbolic backgrounds proposed in [4]. For free fields of this kind, existence of globally defined quasi-free states (or one-particle structures) is discussed. It is shown that such states exist if and only if there is a set of locally defined quasi-free states with sufficiently large domains that satisfy certain compatibility conditions. For the theories that can be constructed on semi-globally hyperbolic spacetime, the dynamics of the theory can be classified with respect to a (generalized notion of) information loss, or lack thereof, via the property of complete dynamics.

Following this general discussion, the introduced concepts are explored for some example spacetimes. A simple but illustrative example is that of the punctured globally hyperbolic spacetime, previously discussed in a context related to evaporating black holes in [5]. The introduced framework allows for a recontextualization of uniqueness in extending linear scalar quantum field theories to these backgrounds. It highlights the importance of regularity conditions such as the Hadamard property in this setting, as well as the relation of this condition to the completeness of the dynamics for theories on these backgrounds. Furthermore, spacetimes with more general ‘gaps’ than

the single puncture are considered and a method for constructing compatible sets of local one-particle structures is given.

Next, black hole evaporation spacetimes are considered. It is observed that the simple construction schemes for compatible sets of one-particle structures cannot directly be applied to the full spacetime, hence existence of globally defined well-behaved two-point functions cannot be established in this way. Nevertheless, one can use the introduced formalism to construct two-point functions on spacetimes that approximate the full black hole evaporation spacetime, leaving out an arbitrary small neighbourhood surrounding the 'evaporation event'. Hence, one can set up a sequence of quantum field theories that, in the purely algebraic sense, have a quantum field theory on the full black hole evaporation spacetime as a limit. The fact that the spaces of two-point functions on this sequence of theories need not have a well-defined limit, hints further in the direction that semi-classical gravity may not be applicable to accurately describe near-singularity physics, even in a heuristic sense. More concretely, input from quantum gravity is crucial to give a consistent description of a black hole evaporation scenario, independently of whether such a description admits information loss or not.

Lastly, some comments are made on how the given framework may be applied to topology-changing spacetimes as well as how this framework compares to other approaches of quantum field theories on non-globally hyperbolic spacetimes, such as those admitting time-like boundaries. Some potential conceptual shortcomings of the approach are also briefly touched upon as part of the concluding remarks.

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Author’s contribution

DWJ is the sole author of this publication, all results obtained in this work are due to DWJ.

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Quantum Fields on Semi-globally Hyperbolic Space-times

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Abstract

We introduce a class of space-times modelling singular events such as evaporating black holes and topology changes, which we dub as semi-globally hyperbolic space-times. On these space-times we aim to study the existence of reasonable quantum field theories. We establish a notion of linear scalar quantum field theories on these space-times, show how such a theory might be constructed and introduce notions of global dynamics on these theories. Applying these constructions to both black hole evaporation and topology changing space-times, we find that existence of algebras can be relatively easily established, while the existence of reasonable states on these algebras remains an unsolved problem.

1 Introduction

In the past sixty years we could witness the emergence of a robust framework to describe quantum field theory on curved space-times. This framework, often referred to as local or algebraic quantum field theory, is versatile enough to study free quantum field theories, perturbative theories or even non-perturbative interacting theories, both in terms of specific integrable models and via an axiomatic approach, on a whole host of background space-times (see [1] for an overview). However, not all background space-times lend themselves particularly well to constructing quantum field theories on them. In most cases where AQFT's are considered, the background space-times are assumed to be globally hyperbolic. This is an assumption on the global causal structure of a background that, not coincidentally, is often also imposed when studying the classical wave equation (or related PDE's) on curved space-times.

While global hyperbolicity is a very convenient property in many contexts, specifically when one is interested in the global dynamics of a theory, every now and then one encounters a physically interesting space-time that is not globally hyperbolic. In some cases one would still like to construct a quantum field theory on these. Examples that may be of interest are space-times with closed time-like curves, i.e. space-times admitting 'time-machines', space-times with time-like (conformal) boundaries, like AdS space-times, topology changing space-times, for instance space-times with dynamically formed wormholes, or space-times with more general naked singularities, such as a fully evaporating black hole space-time. While for some of these space-times it can be said that their physical relevance is mostly speculative, as is the case for wormhole space-times, one cannot ignore nonglobally hyperbolic space-times altogether.

In recent years the space-times that have garnered the most attention when it comes to constructing quantum field theories on them, besides globally hyperbolic space-times that is, are those with time-like boundaries. Examples of work related to this are [2, 3, 4]. No doubt this is partly due to the advent of holographic dualities in physics, most notably the AdS/CFT correspondence which is closely associated with string theory, but also because some well-known classical solutions to the Einstein equations actually admit (singular) time-like boundaries, see for instance a Kerr black hole [5]. One could argue that admitting time-like boundaries is actually only a very minor generalization with regards to global hyperbolicity. In fact many of the geometric properties of globally hyperbolic space-times carry over to 'globally hyperbolic space-times with boundaries' without too much change [6]. However on the side of field theories, both classical and quantum, such a generalization does warrant the introduction of appropriate boundary condition in order to fix time-evolution of the states in a theory.

On the other side of the spectrum, in a sense very far removed from the class of globally hyperbolic space-times, are space-times with closed time-like curves. Quantum fields on space-times such as the space-like cylinder have been considered in [7, 8], which lead to the introduction of a key property that many agree a quantum field on any (non-globally hyperbolic) space-time should adhere to, namely that of F-locality. This property, very loosely speaking, entails that quantum field theories on any space-time should be locally equivalent to a theory on globally hyperbolic space-times. A more recent study of quantum fields on space-times with closed time-like curves can be found in [9]. This work mostly focuses on investigating the D-CTC condition, a model for closed time-like curves in quantum computational network as introduced in [10], in the algebraic framework for quantum fields theory on curved space-times. However, this work also contains an explicit construction of a QFT on Pollitzer space-times, that indeed contain closed time-like curves and the resulting theory is in fact also F-local. While we do not consider space-times with closed time-like curves, F-locality will still be a key feature that we shall adhere to.

So what space-times do we focus our attention on here and why? As mentioned, quantum fields on space-times with time-like boundaries have been relatively well studied (at least in the context of linear scalar fields), and shall therefore not be the focus of this work. Instead, we shall focus on space-times with more discrete (naked) singularities. A main motivation for studying quantum fields on such space-times comes from the supposed structure of evaporating black holes (originating in [11], and more recently studied from the perspective of causal structures in [12]), however we shall in fact study a more general class of space-time for which black hole evaporation space-times are just one example, that we will treat in 4.3. We shall dub this class the semi-globally hyperbolic space-times. Beyond the black hole evaporation space-times, or at least space-times of the conformal class that (semi-classically evolved) evaporating black holes are expected to be a part of, it also contains, for instance, the aforementioned topology changing space-times.

As we will make precise in this paper, to us constructing a (linear scalar) quantum field theory specifically means constructing algebras generated by 'operator valued distributions' on a space-time, satisfying an appropriate equation of motion. While in the case of globally hyperbolic space-times such an approach is in one-to-one correspondence with building an algebra from (symplectic smearings of) solutions to the classical equation of motion (see [13]), this correspondence need no longer hold if one treats more general space-times. This means that the problem of extending classical and quantum field theory to non-globally hyperbolic space-times can become somewhat further separated than on globally hyperbolic space-times.

We rigorously define the class of semi-globally hyperbolic space-times in section 2. In the section that follows, section 3, we propose a notion of an (f-local) linear scalar field theory on these space-times, describe how such a theory can be constructed and discuss how one should interpret notions of global dynamics on these theories. Thereafter, in section 4 and 5 we shall discuss applications of our construction to some example space-times, where we make the further distinction between so-called maximally semi-globally hyperbolic space-times, such as the black hole evaporation space-time, and other semi-globally hyperbolic space-times.

2 Semi-globally hyperbolic space-times

In this section we define the our new class of space-times. However, before we write down this definition, let us recall how globally hyperbolic space-times are defined and what some of their important properties are. Many of these definitions and results, as well as a more general overview of global causal structures, can be found in [14].

Definition 1. *A space-time M (without boundaries) is* globally hyperbolic *if there exists a (smooth) hypersurface $\Sigma \subset M$ such that each inextendible time-like curve in M crosses Σ exactly once. Such a surface Σ is referred to as a (smooth)* Cauchy surface.[1]

There is another way to characterize globally hyperbolic space-times which is often useful.

Proposition 1. *A space-time M is globally hyperbolic if and only if it is* causal *(i.e. contains no closed causal curves) and for each $x, y \in M$ the set $J^+(x) \cap J^-(y)$ is compact.*[2]

Some important features of this class of space-times are as follows.

Proposition 2. *Let M globally hyperbolic with $\Sigma \subset M$ a smooth Cauchy surface, then*

1. *Given any $\Sigma' \subset M$ a further Cauchy surface, then $\Sigma \cong \Sigma'$, i.e. Cauchy surfaces are diffeomorphic.*

2. *There exists a Cauchy time-function, i.e. a continuous function $T : M \to \mathbb{R}$ that strictly increases along each future directed causal curve such that each non-empty level set $T^{-1}(\{t\})$ is a Cauchy surface.*

3. *Given a Cauchy time-function $T : M \to \mathbb{R}$ and $\Sigma_t = T^{-1}(\{t\})$ for some $t \in T(M)$, then $M \equiv T(M) \times \Sigma_t$.*[3]

The existence of a global time-function on a space-time is a feature that goes under the name of *stable causality.* This is one of a hierarchy of causality conditions, of which global hyperbolicity is the strongest. Clearly a stably

[1] One can drop the smoothness condition without changing the class of space-times described by the definition, see [15].

[2] Recall that $y \in J^+(x)$ if there is a future directed causal curve starting at x and ending at y, and that $y \in J^-(x)$ if $x \in J^+(y)$. Furthermore, for a given set $U \subset M$ one defines $J^\pm(U) = \bigcup_{x \in U} J^\pm(x)$. The sets $I^\pm(x)$ and $I^\pm(U)$ are defined similarly, but with time-like curves instead of causal curves.

[3] This is known as Geroch's Theorem [16].

causal space-time does not admit any closed time-like curves, but in fact this property is equivalent to that even when the metric of a stably causal space-time is perturbed (in a way made precise in [14]), no closed time-like curves appear. This is a property we would like to keep in the class of space-times we are considering. Furthermore, as stated we are interested in space-times that, unlike in the case of time-like boundaries, only admit a discrete (i.e. locally finite) number of naked singularities. We can make this precise in the following way.

Definition 2. *Let M a stably causal space-time. We say M is* semi-globally hyperbolic *if there exists a time-function $T : M \to \mathbb{R}$, where for each $a, b \in T(M)$ with $a < b$ there exist a finite set $\{t_i\}_{i=1}^n$ with $t_0 = a$, $t_n = b$ and $t_i < t_{i+1}$ such that for each $i < n$ the (open) space-time $T^{-1}((t_i, t_{i+1}))$ is globally hyperbolic and $T\restriction_{T^{-1}((t_i,t_{i+1}))}$ is a Cauchy time-function. We call such a time-function* semi-Cauchy*.*

Some examples from this class are given by the Penrose diagrams in figure I.1. It should be noted that many semi-globally hyperbolic may be embedded

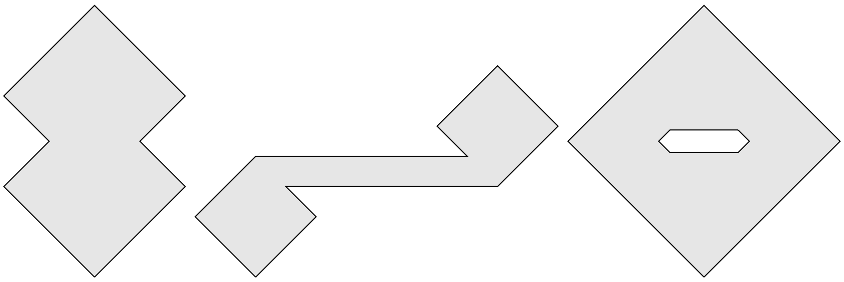

Figure I.1: Some Penrose diagrams of two-dimensional semi-globally hyperbolic space-times

in to globally hyperbolic space-times, although generally not as a causally convex subspace-time. In fact the most simple examples of these are globally hyperbolic space-times from which a point has been removed. These and some similar space-times are discussed in more detail in section 4. We furthermore note that, just as globally hyperbolic space-times (see [17]), the semi-globally hyperbolic space-times form a category where the morphisms are given by causally convex embeddings. To show this, we give an alternative description of semi-globally hyperbolic space-times, which will also prove useful in constructing quantum field theories.

Proposition 3. *A space-time is semi-globally hyperbolic iff for each connected component there is a countable cover $\{M_j : j \in J\}$ of open causally convex* *globally hyperbolic spacetimes such that there is a locally finite total order $\leq$ on J satisfying for $j < j'$*

$$M_j \cap M_{j'} \neq \emptyset \textit{ if and only if } j, j' \textit{ nearest neighbours},$$

$$I^+(M_j \cap M_{j'}) \cap (M_j \cup M_{j'}) \subset M_{j'}, \textit{ and } I^-(M_j \cap M_{j'}) \cap (M_j \cup M_{j'}) \subset M_j.$$

Proof. Without loss of generality assume M is connected. Suppose M is semi-globally hyperbolic and $T : M \to \mathbb{R}$ a semi-Cauchy time function. Note that for any $n \in \mathbb{Z}$ we can find a finite set $J_n = \{t_0, ..., t_m\} \subset [n, n+1]$ such that $t_0 = n$ $t_m = n+1$ and $t_i < t_{i+1}$ such that $T^{-1}((t_i, t_{i+1}))$ causally convex globally hyperbolic. Now define $J = \cup_{n\in\mathbb{Z}} J_n$, which is a countable locally finite totally ordered set $J = \{j_n : n \in \mathbb{Z}\} \subset \mathbb{R}$. For $j_n, j_{n+1} \in J$ nearest neighbours such that $j_n < j_{n+1}$, we set

$$M_{j_n} = D(T^{-1}((j_n, j_{n+1}))) \cap T^{-1}\left(\left(\frac{j_{n-1}+j_n}{2}, \frac{j_{n+1}+j_{n+2}}{2}\right)\right).[4]$$

Note that M_j is causally convex globally hyperbolic, as $D(T^{-1}((j_n, j_{n+1})))$ is causally convex globally hyperbolic and $T^{-1}\left(\left(\frac{j_{n-1}+j_n}{2}, \frac{j_{n+1}+j_{n+2}}{2}\right)\right)$ causally convex. Furthermore $M_{j_n} \cap M_{j_m} \neq \emptyset$ if and only if $|n-m| \leq 1$.

We now show that $\Sigma_{j_n} \subset M_{j_n}$. Suppose $x \in \Sigma_{j_n} = T^{-1}(\{j_n\})$, then clearly

$$x \in T^{-1}\left(\left(\frac{j_{n-1}+j_n}{2}, \frac{j_{n+1}+j_{n+2}}{2}\right)\right).$$

Now, let $\gamma_x : \mathbb{R} \to M$ be an inextendible causal curve through x. Since T is a time function, and hence strictly increasing along causal curves, there must be a $x' \in \gamma_x(\mathbb{R})$ such that $j_n < T(x') < j_{n+1}$, which means γ_x goes through $\Sigma_{T(x')} \subset M_{j_n}$. Since this holds for any time-like curve through x, we see $x \in M_{j_n}$ and hence $\Sigma_{j_n} \subset M_{j_n}$. Since this means that for each $t \in \mathbb{R}$ there is an $n \in \mathbb{Z}$ such that $T^{-1}(\{t\}) \subset M_n$, we see that

$$M = \bigcup_{j\in J} M_j.$$

Observe that $U_n = M_{j_n} \cap M_{j_{n+1}}$ is itself causally convex and hence globally hyperbolic, that $\Sigma_{j_{n+1}}$ is a Cauchy surface for U and that $I^+(U) = U \cup I^+(\Sigma_{j_{n+1}})$. Now suppose

$$x \in I^+(\Sigma_{j_{n+1}}) \cap (M_{j_n} \cup M_{j_{n+1}}),$$

[4]Here $D(U) \subset M$ is the *domain of dependence*, i.e. the set of all points $x \in M$ such that all inextendible causal curves through x intersect $U \subset M$.

let $T(x) > t' > j_{n+1} > t > j_n$, then any inextendible causal curve trough x crosses either $\Sigma_{t'}$ (i.e. $x \in M_{j_{n+1}}$) or it crosses Σ_t (i.e. $x \in M_{j_n}$), but in the latter case by continuity of T we also see that the curve must cross $\Sigma_{t'}$, from which we conclude that

$$I^+(\Sigma_{j_{n+1}}) \cap (M_{j_n} \cup M_{j_{n+1}}) \subset M_{j_{n+1}}.$$

This implies

$$I^+(M_{j_n} \cap M_{j_{n+1}}) \cap (M_{j_n} \cup M_{j_{n+1}}) \subset M_{j_{n+1}},$$

and a similar argument shows that

$$I^-(M_{j_n} \cap M_{j_{n+1}}) \cap (M_{j_n} \cup M_{j_{n+1}}) \subset M_{j_n}.$$

This proves that every semi-globally hyperbolic space-time has a cover with the desired properties.

Now suppose we have a countable cover $\{M_j : j \in J\}$ as in the proposition. Without loss of generality we can assume that $J = \mathbb{Z}$. Observe that $M_n \cap M_{n+1} \neq \emptyset$ is globally hyperbolic and hence we can define for each n a space-like Cauchy surface Σ_n of $M_n \cap M_{n+1}$, which means that $M_n \cap M_{n+1} \subset I^-(\Sigma_n) \cup \Sigma_n \cup I^+(\Sigma_n)$. Now define

$$\tilde{M}_n = M_n \setminus (\Sigma_{n-1} \cup I^-(\Sigma_{n-1}) \cup \Sigma_n \cup I^+(\Sigma_n)).$$

First observe that $(I^-(\Sigma_{n-1}) \cup \Sigma_{n-1}) \cap M_{\subset} M_n$ is a (relatively) closed subset on M_n, as

$$M_n \cap (\Sigma_{n-1} \cup I^-(\Sigma_{n-1})) = (M_n \cap M_{n-1}) \setminus I^+(\Sigma_{n-1}),$$

and $I^+(\Sigma_{n-1})$ is open, which follows from [18, cor. 2.9]. Similarly $(I^+(\Sigma_n) \cup \Sigma_n) \cap M_{\subset} M_n$ is closed. This means in particular that $\tilde{M}_n$ is open. It is also causally convex, as for $a, b \in \tilde{M}_n$ we have $J^+(a) \cap J^-(b) \subset M_n$ compact, and if we suppose $J^+(a) \cap J^-(b) \cap \Sigma_{n-1} \cap I^-(\Sigma_{n-1}) \neq \emptyset$, this means $a \in J^-(\Sigma_{n-1}) \cup \Sigma_{n-1} \subset \overline{I^-(\Sigma_{n-1})} \cup \Sigma_{n-1}$, but as $(I^-(\Sigma_{n-1}) \cup \Sigma_{n-1}) \cap M_n$ is closed in M_n, we see that $a \in \Sigma_{n-1} \cup I^-(\Sigma_{n-1})$, which contradicts $a \in \tilde{M}_n$. A similar contradiction can be derived for $\Sigma_n \cup I^+(\Sigma_n)$ from which we see that $J^+(a) \cap J^-(b) \subset \tilde{M}_n$ compact and hence $\tilde{M}_n$ is globally hyperbolic. Now we can define a Cauchy time-function $T_n : \tilde{M}_n \to (n-1, n)$.

Let $\gamma : (0,1) \to \tilde{M}_n$ a future directed inextendible time-like curve such that $\lim_{\lambda \to 1} \gamma(\lambda) = \Sigma_n$. Clearly $T_n \circ \gamma$ is a bounded monotonically increasing function, so $\lim_{\lambda \to 1}(T_n \circ \gamma)(\lambda) \leq n$ exists. Also, since γ is inextendible and for each $t \in (n-1,n)$ there is a Cauchy surface Σ_t with $T(\Sigma_t) = \{t\}$, then for each $t \in (n-1,n)$ there will be an $\lambda \in (0,1)$ such that $(T \circ \gamma)(\lambda) = t$, hence

$$\lim_{\lambda \to 1} (T_n \circ \gamma)(\lambda) = n.$$

A similar argument can be made for curves approaching Σ_{n-1} and as a result we see that we can define a unique continuous extension $T_n : (\tilde{M}_n \cup \Sigma_{n-1} \cup \Sigma_n) \to [n-1,n]$ satisfying $T_n(\Sigma_n) = \{n\}$ and $T_n(\Sigma_{n-1}) = \{n-1\}$.

From our assumptions we clearly see that for $n \neq m$ we have $\Sigma_n \cap \Sigma_m = \emptyset$. Moreover, suppose $x \in \tilde{M}_n \cap \tilde{M}_m \subset M_n \cap M_m$, then n, m nearest neighbours. Assume without loss of generality that $m = n+1$. It follows that $x \in \Sigma_n$, $x \in I^-(\Sigma_n)$ or $x \in I^+(\Sigma_n)$, where we note that these three options are mutually exclusive. Since $x \in \tilde{M}_n$, this means $x \notin I^+(\Sigma_n) \cup \Sigma_n$, hence $x \in I^-(\Sigma_n)$, so $x \notin \tilde{M}_{n+1}$, which is a contradiction. Hence we see that $\tilde{M}_n \cap \tilde{M}_m = \emptyset$. What follows is that

$$M = \bigcup_{n \in \mathbb{Z}} \tilde{M}_n \cup \Sigma_n,$$

is a disjoint union and we can uniquely extend all T_n's to a semi-Cauchy time-function $T : M \to \mathbb{R}$ such that $T\restriction_{\tilde{M}_n} = T_n$. This implies that M is semi-globally hyperbolic. □

Since for each causally convex $U \subset M$ for $M = \bigcup_{j \in J} M_j$ connected and semi-globally hyperbolic with the cover satisfying the properties of proposition 3, the cover $U = \bigcup_{j \in J}(U \cap M_j)$ satisfies the same properties (for each connected component of U). The result below follows.

Corollary. *Let M semi-globally hyperbolic and $U \subset M$ causally convex. Then U is also semi-globally hyperbolic.*

As these aforementioned covers play a crucial role in the rest of this paper, we ought to give them a name.

Definition 3. *Let M semi-globally hyperbolic with a cover $\{M_j : j \in J\}$ satisfying the properties of proposition 3, we say this is a* time-ordered cover.

Given the examples in figure I.1, we can draw in (some choice of) a time-ordered cover as can be seen in figure I.2. These time-ordered covers are in general not unique, but for a certain subclass of semi-globally hyperbolic space-times we can associate a preferred cover.

Definition 4. *We say a space-time M is* maximally semi-globally hyperbolic *if it is semi-globally hyperbolic and there is a time-ordered cover $\{M_j : j \in J\}$*

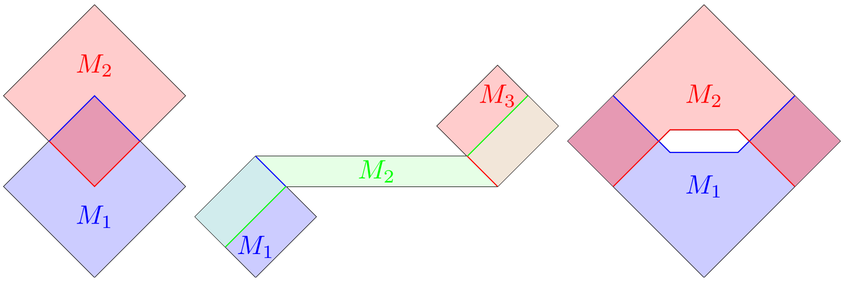

Figure I.2: Some Penrose diagrams of two-dimensional semi-globally hyperbolic space-times with time-ordered covers drawn in

of connected sub-spacetimes M_j*, such that for each connected causally convex globally hyperbolic* $U \subset M$ *there is a* $j \in J$ *such that* $U \subset D(M_j)$ *and such that* $M_j \subset D(M_{j'})$ *implies* $D(M_j) = D(M_{j'})$*. We refer to the cover* $\{D(M_j) : j \in J\}$ *as the* maximal cover.

Proposition 4. *The maximal cover on a maximally semi-globally hyperbolic space-time is unique.*

Proof. Suppose $\{D(M_j) : j \in J\}$ and $\{D(M_k) : k \in K\}$ both maximal covers, then for any $j \in J$ the space-time M_j is connected causally convex globally hyperbolic and hence there is a $k \in K$ such that $M_j \subset D(N_k)$, similarly there is a $j' \in J$ such that $N_k \subset D(M_{j'})$, which implies $D(M_j) = D(M_{j'})$, from which is also follows that $D(N_k) = D(M_j)$. Hence for each $j \in J$ there is a $k \in K$ such that $D(M_j) = D(N_k)$ and vice versa. □

We have now characterized the class of space-times on which we shall attempt to define linear scalar quantum field theories. It is worth mentioning again that one subclass of these space-times that we will treat in section 4.3 are the (spherically symmetric) black hole evaporation space-times. These space-times are characterized by their (symmetry reduced) Penrose diagram, most famously drawn in [11]. As can be seen in figure I.3, these space-times are in fact maximally semi-globally hyperbolic.

3 Linear scalar quantum fields on semi-globally hyperbolic space-times

For our purposes, (real) linear scalar quantum field theory is a quantization of a classical field satisfying the equation of motion

$$(\Box - V)\phi = 0. \tag{1}$$

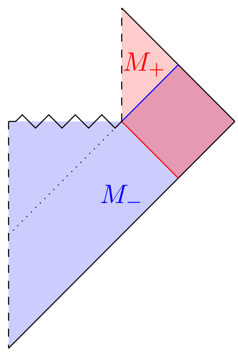

Figure I.3: Hypothesised Penrose diagram of a fully evaporating spherically symmetric black hole with its maximal cover

Here $\Box = \nabla^\mu \nabla_\mu$ with ∇ the Levi-Civita connection on a given background space-time and V some potential.[5] If we want this potential V to be locally covariant, it should take the form $V = m + \xi R$, with m the mass of the field and ξ a dimensionless coupling of the field to the Ricci scalar R. For the purposes of this paper we consider m and ξ to be fixed. The construction of the linear scalar quantum field theory on globally hyperbolic space-times, including some important features of this theory, are reviewed in appendix A.

3.1 Algebras from states

Based on the qualities of the real linear scalar quantum field on globally hyperbolic space-times, we set out some list of requirements that we want our quantum field theories on semi-globally hyperbolic space-times to satisfy. It should be noted that we do not assume that every semi-globally hyperbolic space-time M admits a sensible quantum field theory. Luckily, we can take a page from [8] to get us started on some very minimal requirements for a free scalar quantum field theory on any space-time. So for M a non-globally hyperbolic space-time, we require that any real scalar quantum field theory (i.e. some unital *-algebra $\mathcal{A}(M)$) has the following properties.

- *Net structure*: There is some set $\mathcal{O}$ of open neighbourhoods in M containing at least all relatively compact subspaces, such that for each $U \in \mathcal{O}$ there is an algebra

$$\mathcal{A}(M; U) \subset \mathcal{A}(M),$$

[5] We take the metric to have $(- + + +)$ signature.

that in itself defines a quantum field theory on U, and where for any $U, V \in \mathcal{O}$ with $U \subset V$ we have

$$\mathcal{A}(M; U) \subset \mathcal{A}(M; V).$$

- *F-locality*: For each $x \in U \in \mathcal{O}$ there is a (a priori not necessarily causally convex) globally hyperbolic $N \in \mathcal{O}$ with $x \in N \subset U$ such that

  $$\mathcal{A}(M; N) \cong \mathcal{A}(N),$$

  via a net-preserving *-isomorphism, with $\mathcal{A}(N)$ the algebra of definition 13.

The net structure is essential to localize observables of a quantum field theory to regions in a space-time. F-locality on the other hand tells us that in some arbitrarily small globally hyperbolic neighbourhood our quantum field theory matches the standard theory on globally hyperbolic space-times (for some given potential V). This assumption can be understood from the fact that locally we are not able to discern the global causal structure of a space-time, so one would expect that at this local level one can also not distinguish between a quantum field theory on globally hyperbolic and non-globally hyperbolic space-times, which is fully in keeping with the traditions of local quantum field theory. That being said, one can argue that on the basis of this logic, the theory should match that of definition 13 on any globally hyperbolic region, and not just on some arbitrarily small one. However in the context that F-locality was first discussed, namely in the presence of closed time-like curves, such a requirement is too restrictive to even begin to construct a quantum field theory [19]. Nevertheless, on our semi-globally hyperbolic space-times we can often do a bit better, especially on maximally semi-globally hyperbolic space-times. To keep some further bounds on what kind of theories one would deem acceptable, we also introduce an additional requirement.

- The algebra $\mathcal{A}(M)$ can be generated by elements of the form $\hat{\phi}(f)$ for $f \in \mathcal{D}(M)$ such that for $f, g \in \mathcal{D}(M)$, the commutator $[\hat{\phi}(f), \hat{\phi}(g)] \in \mathcal{A}(M)$ is in the center of the algebra.

In principle one could allow theories with more involved commutation relations, but we deem this a natural generalization of the fact that in the globally hyperbolic case these commutators are always a multiple of the identity. At the very least this property requires that the commutation relation of our algebra is always specified to some degree, unlike for instance in the approach set out in [4]. As an upshot of this restriction, one can still sensibly define quasi-free states on such algebras.

Let us capture all the required features in the following definition for linear scalar fields on semi-globally hyperbolic space-times.

Definition 5. *Given a semi-globally hyperbolic space-time M with time-ordered cover $\{M_i \subset M\}_{i \in I}$, we say a *-algebra $\mathcal{A}(M)$ is a* scalar field algebra *on M if there is a surjective *-homomorphism $\varphi : \mathcal{B}(M) \to \mathcal{A}(M)$, with $\mathcal{B}(M)$ as in definition 13, where φ defines a net structure*

$$\mathcal{A}(M;U) = \varphi(\mathcal{B}(M;U))$$

*such that for each $i \in I$ there is a *-isomorphism $\iota_i : \mathcal{A}(M_i) \to \mathcal{A}(M;M_i)$, such that given the natural $\iota_i' : \mathcal{B}(M_i) \to \mathcal{B}(M)$ and surjective *-homomorphism $\varphi_i : \mathcal{B}(M_i) \to \mathcal{A}(M_i)$ (via the quotient of definition 13), the following diagram commutes*

$$\begin{array}{ccc} \mathcal{B}(M) & \xrightarrow{\varphi} & \mathcal{A}(M) \\ {\scriptstyle \iota_i'}\uparrow & & {\scriptstyle \iota_i}\uparrow \\ \mathcal{B}(M_i) & \xrightarrow{\varphi_i} & \mathcal{A}(M_i), \end{array}$$

and where, denoting for $f \in \mathcal{D}(M)$

$$\hat{\phi}(f) = \varphi(\hat{\psi}(f)),$$

we require that for all $f, g, h \in \mathcal{D}(M)$

$$[[\hat{\phi}(f), \hat{\phi}(g)], \hat{\phi}(h)] = 0.$$

Note that the fact that commutators $[\hat{\phi}(f), \hat{\phi}(g)]$ are part of the center of the algebra also allow us to construct a Weyl-like C*-algebra $\mathfrak{A}(M)$ associated with the *-algebra $\mathcal{A}(M)$. Namely, as the group C*-algebra of $Z_{s.a.}(\mathcal{A}(M)) \times \hat{\phi}(\mathcal{D}(M))$ with $Z_{s.a.}(\mathcal{A}(M))$ the self-adjoint elements of the center of the algebra $\mathcal{A}(M)$ and the group operation defined by

$$\left(a, \hat{\phi}(f)\right) \cdot \left(b, \hat{\phi}(g)\right) = \left(a + b + \frac{i}{2}[\hat{\phi}(f), \hat{\phi}(g)], \hat{\phi}(f+g)\right).$$

If for $N \subset M$ one defines $\mathfrak{A}(M;N) \subset \mathfrak{A}(M)$ as the smallest C*-subalgebra containing all elements $\{0\} \times \hat{\phi}(\mathcal{D}(N)) \subset \mathfrak{A}(M)$, then we see that for each $i \in I$

$$\mathfrak{A}(M;M_i) \cong \mathfrak{A}(M_i),$$

via a net-preserving isomorphism, with $\mathfrak{A}(M_i)$ the standard Weyl-algebra on the globally hyperbolic space-time M_i. We conclude that from a scalar field algebra $\mathcal{A}(M)$ we can construct an F-local net of C*-algebras on M.

As alluded to earlier, we have in fact imposed a stronger notion of F-locality on these quantum field theories than what is usually considered. One comment we should make here is that this definition depends on the choice of time-ordered cover (or via proposition 3 a choice of semi-Cauchy time-function). It is a priori not guaranteed that a scalar field algebra with respect to some time-ordered cover will also be a scalar field algebra with respect to any other time-ordered cover. In the case of maximally semi-globally hyperbolic space-times this situation is less dire, as here one most naturally defines linear scalar algebras with respect to the maximal cover. This then guarantees that such an algebra is a linear scalar algebra with respect to any cover. Nevertheless, with our mind set on some applications in section 5, we don't want to restrict our definition to just maximally semi-globally hyperbolic space-times.

Having a *-algebra with a net structure is a good start, but of course one also is interested in what kind of states such an algebra admits. A particularly central question is whether a linear scalar algebra actually admits states in the first place. While the C*-algebra $\mathfrak{A}(M)$ associated with a scalar field algebra $\mathcal{A}(M)$ will always admit states (see [20, Lemma 2.3.23]), this does not mean that these states correspond to states on $\mathcal{A}(M)$, as n-point function of an arbitrary state on $\mathfrak{A}(M)$ are generally not defined. Since n-point functions are crucial objects in many uses of quantum field theory, especially those satisfying the Hadamard property (see [21]), we view existence of n-point functions as imperative for any reasonable scalar field algebra. This requirement is the starting point of the construction in the rest of this section, where we particularly focus on 2-point functions, quasi-free states and one-particle structures, existence of which are of course equivalent to the existence of n-point functions for all n.

A gluing procedure of one-particle structures

As mentioned above, we shall be constructing quantum field theories on semi-globally hyperbolic space-times from (extended) one particle structures. The definition of a one-particle structure is recalled in definition 16.

Definition 6. *For a semi-globally hyperbolic space-time M with time-ordered cover $\{M_j : j \in J\}$ we say (K, H) with H a Hilbert space and $K : \mathcal{D}(M) \to H$*

a real linear map is an extended one-particle structure *if*

$$\overline{K(\mathcal{D}(M)) + iK(\mathcal{D}(M))} = H,$$

and for each $j \in J$ the pair (K_j, H_j) with

$$K_j = K\restriction_{\mathcal{D}(M_j)},$$

and

$$H_j = \overline{K(\mathcal{D}(M_j)) + iK(\mathcal{D}(M_j))},$$

form a one-particle structure on $(\mathcal{D}(M_j), \sigma_{M_j})$, with σ_{M_j} the standard presyplectic form on $\mathcal{D}(M_j)$ given the wave eq. (1)*, as defined in theorem 12 in the appendix.*

Again here the choice of time-ordered cover influences what one would call an extended one-particle structure, but in any case we have the following.

Proposition 5. *Given the assumptions of the definition above, an extended one-particle structure (K, H) satisfies*

$$K \circ (\Box - V) = 0.$$

Proof. Note that given an open cover $\{M_j : j \in J\}$ and $f \in \mathcal{D}(M)$, we can always find a finite $J' \subset J$ with for each $j \in J'$ an $f_j \in \mathcal{D}(M_j)$ such that $f = \sum_{j \in J'} f_j$. This means

$$K((\Box - V)f) = \sum_{j \in J'} K((\Box - V)f_j) = \sum_{j \in J'} K_j((\Box - V)f_j) = \sum_{j \in J'} 0 = 0.$$

$\Box$

For each extended one-particle structure one has a (real) pre-inner product μ and pre-symplectic structure σ on $\mathcal{D}(M)$ via

$$\mu(f, g) = Re(\langle Kf, Kg \rangle),$$

$$\sigma(f, g) = 2Im(\langle Kf, Kg \rangle).$$

Here we note that for any $j \in J$

$$\sigma\restriction_{\mathcal{D}(M_j)^2} = \sigma_{M_j},$$

with σ_{M_j} the natural symplectic structure as defined in theorem 12.

In general these one-particle structures will not be 'god-given' and one has to construct them. One way to do this is via compatible locally defined one-particle structures. The main result of this section is therefore as follows.

Theorem 6. *A semi-globally hyperbolic space-time M with time-ordered cover $\{M_j : j \in J\}$ admits an extended one-particle structure if and only if there is a chain of one-particle structures $\{(K_j, H_j) : j \in J\}$, one for each globally hyperbolic patch of the cover, such that for each $j < j'$ nearest neighbours we have for $f, g \in \mathcal{D}(M_j \cap M_j')$ that*

$$\langle K_j f, K_j g\rangle_j = \langle K_{j'} f, K_{j'} g\rangle_{j'}.$$

We prove this statement by explicitly constructing such an extended one-particle structure from a given chain via a procedure that we will refer to as a *minimal gluing.*

To describe the minimal gluing of one-particle structure on patches of a general semi-globally hyperbolic space-time, we first treat the simpler case of a space-time that is just the union of two globally hyperbolic space-times.

Definition 7. *Let M a space-time and $M_1, M_2 \subset M$ causally convex globally hyperbolic such that they form an open cover of M. Suppose for each $j \in \{1, 2\}$ we have a one-particle structure (K_j, H_j) for the pre-symplectic space $(\mathcal{D}(M_j), \sigma_j)$ such that for $f, g \in \mathcal{D}(M_1 \cap M_2)$*

$$\langle K_1 f, K_1 g\rangle_1 = \langle K_2 f, K_2 g\rangle_2,$$

we say these one-particle structures form a compatible pair*.*

Now let p_j the Hilbert space projection of H_j onto

$$O_j = \overline{K_j(\mathcal{D}(M_1 \cap M_2)) + iK_j(\mathcal{D}(M_1 \cap M_2))},$$

and $U : O_1 \to O_2$ the unitary such that $UK_1 f = K_2 f$ for each $f \in \mathcal{D}(M_1 \cap M_2)$. We define the minimally glued one-particle structure *$(\tilde{K}, \tilde{H})$ with*

$$\tilde{H} = H_1 \oplus H_2 / \{(\psi_1, \psi_2) : \langle\psi_1, \psi_1\rangle_1 + \langle\psi_2, \psi_2\rangle_2 + \langle\psi_1, U^* p_2 \psi_2\rangle_1 + \langle\psi_2, U p_1 \psi_1\rangle_2 = 0\},$$

where we define the inner product on $\langle ., .\rangle$ on $\tilde{H}$ as

$$\langle[(\psi_1, \psi_2)], [(\phi_1, \phi_2)]\rangle = \langle\psi_1, \phi_1\rangle_1 + \langle\psi_2, \phi_2\rangle_2 + \langle\psi_1, U^* p_2 \phi_2\rangle_1 + \langle\psi_2, U p_1 \phi_1\rangle_2,$$

and with $\tilde{K} : \mathcal{D}(M) \to \tilde{H}$ defined by

$$\tilde{K}(f_1 + f_2) = [(K_1 f_1, K_2 f_2)],$$

for $f_i \in \mathcal{D}(M_i)$.

For this construction of minimal gluing, we introduce the notation

$$(\tilde{K}, \tilde{H}) = (K_1, H_1) \| (K_2, H_2).$$

In the following lemma we prove that the definitions above are well-defined

Lemma 7. *In the definition above $\langle ., . \rangle$ is a well-defined inner product on the Hilbert space $\tilde{H}$ and $\tilde{K} : \mathcal{D}(M) \to \tilde{H}$ is a well-defined real linear map.*

Proof. Starting with the claims on the inner product, we first note that for $(\psi_1, \psi_2), (\phi_1, \phi_2) \in H_1 \oplus H_2$ the map

$$((\psi_1, \psi_2), (\phi_1, \phi_2)) \mapsto \langle \psi_1, \phi_1 \rangle_1 + \langle \psi_2, \phi_2 \rangle_2 + \langle \psi_1, U^* p_2 \phi_2 \rangle_1 + \langle \psi_2, U p_1 \phi_1 \rangle_2$$

is a positive semi-definite sesquilinear map (i.e. it is a pre-inner product). This follows immediately from the fact that we can rewrite

$$\begin{aligned} &\langle \psi_1, \phi_1 \rangle_1 + \langle \psi_2, \phi_2 \rangle_2 + \langle \psi_1, U^* p_2 \phi_2 \rangle_1 + \langle \psi_2, U p_1 \phi_1 \rangle_2 = \\ &\langle p_1^\perp \psi_1, p_1^\perp \phi_1 \rangle_1 + \langle p_2^\perp \psi_2, p_2^\perp \phi_2 \rangle_2 + \langle U p_1 \psi_1 + p_2 \psi_2, U p_1 \phi_1 + p_2 \phi_2 \rangle_2. \end{aligned}$$

We can now recognize that $\tilde{H}$ is the semi-norm reduction of $H_1 \oplus H_2$ with respect to the pre-inner product above, hence $\langle ., . \rangle$ is well-defined.

For $\tilde{H}$ to form a Hilbert space with the inner product $\langle ., . \rangle$, we need to show it is complete. Suppose $[(\psi_{1,n}, \psi_{2,n})]$ to form a Cauchy sequence in $\tilde{H}$. Using the rewritten form of the inner product, we can see that $p_1^\perp \psi_{1,n}$ is Cauchy in $p_1^\perp H_1$, $p_2^\perp \psi_{2,n}$ in $p_2^\perp H_2$ and $U p_1 \psi_1 + p_2 \psi_2$ in O_2. Therefore we can define $\psi_1 = \lim_{n\to\infty} p_1^\perp \psi_{1,n} \in p_1^\perp H_1$, $\psi_2 = \lim_{n\to\infty} p_2^\perp \psi_{2,n} \in p_2^\perp H_2$ and $\psi_O = \lim_{n\to\infty} U p_1 \psi_1 + p_2 \psi_2 \in O_2$, and define $\Psi = [(\psi_1, \psi_O + \psi_2)]$. Using that $p_i \psi_i = 0$, we now see that

$$\begin{aligned} &\lim_{n\to\infty} \| [(\psi_{1,n}, \psi_{2,n})] - [(\psi_1, \psi_O + \psi_2)] \| = \\ &\lim_{n\to\infty} \| p_1^\perp (\psi_{1,n} - \psi_1) \|_1 + \| p_2^\perp (\psi_{2,n} - \psi_O - \psi_2) \|_2 \\ &\qquad + \| U p_1 (\psi_{1,n} - \psi_1) + p_2 (\psi_{2,n} - \psi_O - \psi_2) \|_2 = \\ &\lim_{n\to\infty} \| p_1^\perp \psi_{1,n} - \psi_1 \|_1 + \| p_2^\perp \psi_{2,n} - \psi_2 \|_2 + \| U p_1 \psi_{1,n} + p_2 \psi_{2,n} - \psi_O \|_2 = 0, \end{aligned}$$

from which we conclude that $\tilde{H}$ is complete.

Now to show that $\tilde{K}$ is well defined, first observe that for any $f \in \mathcal{D}(M)$ there exist $f_i \in \mathcal{D}(M_i)$ such that $f = f_1 + f_2$, as can for instance be seen using partitions of unity. Now suppose $f_1 + f_2 = g_1 + g_2$ for $g_i \in \mathcal{D}(M_i)$, observe that $f_1 - g_1 = g_2 - f_2 \in \mathcal{D}(M_1 \cup M_2)$. We now see that

$$\begin{aligned} &\| [(K_1 f_1, K_2 f_2)] - [(K_1 g_1, K_2 g_2)] \| = \| [(K_1 (f_1 - g_1), K_2 (f_2 - g_2))] \| = \\ &\| U K_1 (f_1 - g_1) + K_2 (f_2 - g_2) \|_2 = \| K_2 (f_1 - g_1 + f_2 - g_2) \|_2 = \| K_2 0 \|_2 = 0. \end{aligned}$$

Hence, $\tilde{K}$ is well defined. $\square$

Using very similar arguments as above, we get the following.

Corollary. *$\tilde{K}(D(M)) + i\tilde{K}(D(M))$ is dense in $\tilde{H}$.*

Since the maps $\tilde{K}\restriction_{\mathcal{D}(M_i)}$ define one-particle structures equivalent to K_i, the minimal gluing $(\tilde{K}, \tilde{H})$ indeed defines an extended one-particle structures. However generally this extension is not unique. This fact can be traced back to the fact that in our construction of the minimal gluing, we defined the inner product on $\tilde{H}$ such that for $\psi_1 \in p_1^\perp H_1$ and $\phi_2 \in p_2^\perp H_2$ we have

$$\langle [(\psi_1, 0)], [(0, \phi_2)] \rangle = 0.$$

In the end this is a somewhat arbitrary choice and in principle there can be many more extensions consistent with the same pair of one-particle structures. However, as $\langle ., . \rangle$ should still define an inner product on $\tilde{H}$, the cross-terms like $\langle [(\psi_1, 0)], [(0, \phi_2)] \rangle$ cannot just be chosen fully arbitrarily. Setting these cross-terms to zero is arguably the most simple, or minimal, consistent choice, which is in fact why we chose to call this particular construction the *minimal* gluing.[6]

Until now we have only considered space-times that were built from two globally hyperbolic patches. Let us now generalize our gluing procedure to arbitrary semi-globally hyperbolic space-times.

Definition 8. *Let $M = \bigcup_{j \in J} M_j$ be semi-globally hyperbolic with time-ordered cover. Let (K_j, H_j) be one-particle structures that are pairwise compatible, we then refer to $\{((K_j, H_j)) : j \in J\}$ as a* compatible chain *of one-particle structures. We now define $(\tilde{K}, \tilde{H}) = \|\{((K_j, H_j)) : j \in J\}$ as follows. Let $j, j' \in J$ with $j < j'$, for the interval $[j, j']$ we define $(\tilde{K}_{[j,j']}, \tilde{H}_{[j,j']})$ inductively via*

$$(\tilde{K}_{[j,j']}, \tilde{H}_{[j,j']}) = (\tilde{K}_{[j,j'] \setminus \{j'\}}, \tilde{H}_{[j,j'] \setminus \{j'\}}) \| (K_{j'}, H_{j'}).$$

Now for $[j, j'] \subset [k, k'] \subset J$ we define $\varphi_{[j,j'],[k,k']} : \tilde{H}_{[j,j']} \to \tilde{H}_{[k,k']}$ as the unique isometric embedding such that for $f \in \mathcal{D}\left(\bigcup_{l \in [j,j']} M_l\right)$ we have

$$\varphi_{[j,j'],[k,k']} \tilde{K}_{[j,j']} f = \tilde{K}_{[k,k']} f.$$

We now define $\tilde{H}$ as the direct limit of the directed set $\{\tilde{H}_{[j,j']}; j < j'\}$, i.e.

$$\tilde{H} = \left. \bigsqcup_{j,j' \in J, j < j'} \tilde{H}_{[j,j']} \middle/ \sim \right.$$

[6]Uniqueness of the extension is guaranteed if one of the two one-particle structures, or rather their associated quasi-free states, satisfy the Reeh-Schlieder property (see for instance [22]), or at least satisfy it with respect to $M_1 \cap M_2$. In fact suppose (K_1, H_1) satisfies the Reeh-Schlieder property, this means that $p_1^\perp H_1 = \{0\}$.

where $(H_{[j,j']}, \psi_{[j,j']}) \sim (H_{[k,k']}, \psi_{[k,k']})$ *if there are* $l, l' \in J$ *such that* $[j, j'] \cup [k, k'] \subset [l, l']$ *and* $\varphi_{[j,j'],[l,l']}\psi_{[j,j']} = \varphi_{[k,k'],[l,l']}\psi_{[k,k']}$. *This also yields an natural isometric embedding* $\varphi_{[j,j'],J} : H_{[j,j']} \to H$.

For $f \in \mathcal{D}(M)$, *take some* $[j, j'] \subset J$ *such that* $supp(f) \in \bigcup_{l\in[j,j']} M_l$, *and now define*

$$\tilde{K}f = \varphi_{[j,j'],J}\tilde{K}_{[j,j']}f.$$

Applying this definition to a slightly more simple setting, we get the following result from straightforward calculation.

Proposition 8. *Let* M *a semi-globally hyperbolic space-time* M *with time-ordered cover* $M = \bigcup_{j=0}^n M_i$ *and a minimal extension* $(\tilde{K}, \tilde{H}) = \|_{j=0}^n(K_i, H_i)$ *defined from a compatible chain of one-particle structures as in definition 8, define*

$$p_j : H_j \to \overline{K_j(\mathcal{D}(M_j \cap M_{j-1})) + iK_j(\mathcal{D}(M_j \cap M_{j-1}))},$$

as the projector w.r.t the inner product $\langle ., . \rangle_j$ *and*

$$\begin{aligned} U_j :& \overline{K_j(\mathcal{D}(M_j \cap M_{j-1})) + iK_j(\mathcal{D}(M_j \cap M_{j-1}))} \\ &\to \overline{K_{j-1}(\mathcal{D}(M_j \cap M_{j-1})) + iK_{j-1}(\mathcal{D}(M_j \cap M_{j-1}))} \end{aligned}$$

the natural unitary map, we find for $f \in \mathcal{D}(M_0)$ *and* $g \in \mathcal{D}(M_n)$

$$\langle \tilde{K}f, \tilde{K}g \rangle = \langle K_0 f, U_1 p_1 ... U_n p_n K_n g \rangle_0.$$

Similarly, defining $p'_j : H_{j-1} \to \overline{K_{j-1}(\mathcal{D}(M_j \cap M_{j-1})) + iK_{j-1}(\mathcal{D}(M_j \cap M_{j-1}))}$ *as the projector w.r.t.* $\langle ., . \rangle_{j-1}$, *we find*

$$\langle \tilde{K}f, \tilde{K}g \rangle = \langle U_n^* p'_n ... U_1^* p'_1 K_0 f, K_n g \rangle_n.$$

Here we see explicitly that the fact that our covers admit some natural time-ordering matters in the construction, as projectors p_i and p_j, even when extended to $\tilde{H}$, generally do not commute, hence we need some (geometric) input to decide on the ordering.

Constructing the algebra from one-particle structures

Our goal of this section is as follows. Given a set of extended one-particle structures on a semi-globally hyperbolic space-time $M = \bigcup_{j\in J} M_j$, we want to construct the smallest scalar field algebra $\mathcal{A}(M)$ such that a given set of one-particle structures extend to Fock-space representations of this algebra.

For a single extended one particle structure, we define the associated scalar field algebra in the following way.

Definition 9. *Let M semi-globally hyperbolic and $\{M_j : j \in J\}$ the ordered cover. Given (K, H) an extended one-particle structure, we define the scalar field algebra $\mathcal{A}_{(K,H)}(M)$ as follows. Let $\mathcal{B}(M)$ the the pre-field algebra of linear observables on M as defined in 13. Now let $\mathcal{J}_{(K,H)} \subset \mathcal{B}(M)$ the smallest ideal such that for each $f, g \in \mathcal{D}(M)$ we have*

$$[\hat{\psi}(f), \hat{\psi}(g)] - i\sigma(f, g) \in \mathcal{J}_{(K,H)},$$

and for each $f \in \mathcal{D}(M)$ satisfying

$$\mu(f, f) = 0,$$

we have $\psi(f) \in \mathcal{J}_{(K,H)}$. We define

$$\mathcal{A}_{(K,H)}(M) = \mathcal{B}(M)\Big/\mathcal{J}_{(K,H)} .$$

That this algebra satisfies definition 5, can be seen from the following lemma.

Lemma 9. *Let M, $\{M_j : j \in J\}$, (K, H) and $\mathcal{A}_{(K,H)}(M)$ as in definition 9. For $j \in J$, let $\mathcal{J}_j \subset \mathcal{B}(M_j)$ the ideal of definition 13 and $\iota'_j : \mathcal{B}(M_j) \to \mathcal{B}(M; M_j)$ the natural isomorphism. Then*

$$\mathcal{J}_{(K,H)} \cap \mathcal{B}(M; M_j) = \iota'_j(\mathcal{J}_j).$$

Proof. Suppose

$$a \in \mathcal{J}_{(K,H)} \cap \mathcal{B}(M; M_j) \subset \mathcal{B}(M; M_j),$$

this is equivalent to that $a = \sum_{n=0}^{N} a_n$ where for each n there are $b_n, c_n \in \mathcal{B}(M; M_j)$ such that either

1. $f, g \in \mathcal{D}(M)$ with $\text{supp}(f), \text{supp}(g) \subset M_j$ such that

$$a_n = b_n([\hat{\psi}(f), \hat{\psi}(g)] - i\sigma(f, g))c_n$$

   or

2. $f \in \mathcal{D}(M)$ with $\text{supp}(f) \subset M_j$ and $\mu(f, f) = 0$ such that

$$a_n = b_n\hat{\psi}(f)c_n.$$

In the first case, we clearly see that $a_n \in \iota'_j(\mathcal{J}_j)$, as we know that $\text{supp}(f), \text{supp}(g) \subset M_j$

$$\sigma(f, g) = \sigma_{M_j}(f, g).$$

In the second case, observe that

$$|\sigma_{M_j}(f,g)|^2 \leq 4\mu(f,f)\mu(g,g).$$

It follows that $\mathrm{supp}(f) \subset M_j$ and $\tilde{\mu}(f,f) = 0$ imply that $\sigma_{M_j}(f,g) = 0$ for all $g \in \mathcal{D}(M; M_j)$. This implication also goes the other way, as we know that if $\sigma_{M_j}(f,g) = 0$ for all $g \in \mathcal{D}(M; M_j)$, then $f \in (\Box - V)\mathcal{D}(M; M_j)$ and hence $\mu(f,f) = 0$.

We conclude that $a \in \mathcal{J}_{(K,H)} \cap \mathcal{B}(M; M_j)$ if and only if $a = \sum_n a_n$ with $a_n \in \iota'_j(\mathcal{J}_j)$, which is in turn equivalent to $a \in \iota'_j(\mathcal{J}_j)$. $\Box$

It should be clear that the quantum field algebra $\mathcal{A}_{(K,H)}(M)$ admits a quasi-free state ω for which the two-point function is given by μ via

$$\omega\left(\hat{\phi}_{(K,H)}(f)\hat{\phi}_{(K,H)}(g)\right) = \langle Kf, Kg\rangle = \mu(f,g) + \frac{i}{2}\sigma(f,g).$$

In fact we can easily lift the discussion following definition 17 to this algebra to see that the GNS representation associated with the state above also yields a faithful Fock-space representation where the one-particle Hilbert space matches H.

We have seen how, assuming the fact that a semi-globally hyperbolic space-time admits a compatible chain of one-particle structures, we can construct a quantum field theory on this space-time that admits a Fock-space representation with a one-particle Hilbert space that corresponds to the gluing of this particular compatible chain of one-particle structures. However in general there may be many compatible chains that can be extended in several ways and one may not want to select a preferred one. We will reflect on this further when we treat some example space-times. For now suppose that we have some set E consisting of numerous extended one-particle structures, we wish to construct an algebra that for each $(K,H) \in E$ admits a quasi-free state ω with matching two-point function and Fock-space representation. Such an algebra can be easily constructed using these Fock space representations.

Definition 10. *Let M semi-globally hyperbolic and $\{M_j : j \in J\}$ the ordered cover. For a set E consisting of extended one-particle structures, let $(\mathfrak{H}_{(K,H)}, \pi_{(K,H)})$ be the Fock space representation of $\mathcal{A}_{(K,H)}(M)$ associated with $(K,H) \in E$. We now define $\mathcal{A}_E$ the algebra generated by operators $\{\hat{\phi}_E(f) : f \in \mathcal{D}(M)\}$ on*

$$\mathfrak{H}_E = \bigoplus_{(K,H)\in E} \mathfrak{H}_{(K,H)},$$

defined via

$$\hat{\phi}_E(f)\left(\Psi_{(K,H)}\right)_{(K,H)\in E} = \left(\pi_{(K,H)}\left(\hat{\psi}_{(K,H)}(f)\right)\Psi_{(K,H)}\right)_{(K,H)\in E}.$$

Clearly, this algebra is a scalar field algebra in the sense of definition 5. It is tempting to view the choice of which one-particle structures one uses to define the theory as some choice of boundary condition. However, while these are not two completely unrelated choices, as we will see for instance in section 4.1, not every choice of a one-particle structure corresponds to a particular boundary condition. Nevertheless, there is an intimate relationship between the global dynamics of the theory and the set E. This is something we make precise below.

3.2 Dynamics on scalar field algebras

Recall that quantum field theories on globally hyperbolic space-times ought to satisfy the time-slicing axiom. This can be seen as quantum field theoretical version of theorem 11, i.e. the fact that there is some well-posed global dynamics. We wish to also have a notion of global dynamics on our scalar field algebras. This is given by the definition below.

Definition 11. *Given a semi-globally hyperbolic space-time with time-ordered cover $M = \cup_{j\in J} M_j$, we say a quantum field theory $\mathcal{A}(M)$ is* past predictive *if for each $j \in J$ we have*

$$\mathcal{A}(M; M_j) = \mathcal{A}(M; \cup_{j'\leq j} M_{j'}).$$

Similarly it is future predictive *if*

$$\mathcal{A}(M; M_j) = \mathcal{A}(M; \cup_{j'\geq j} M_{j'}).$$

We say a theory has complete dynamics *if the theory is both past and future predictive.*[7]

Here we should stress once again the choice of time-ordered cover matters for this definition. However here this is very natural, as we have seen in proposition 3 that the time-ordered cover relates to a choice of semi-Cauchy time-function and hence to a global notion of time. Clearly what notion of time one adheres may play a role in what one would consider the global

[7]The notion of past predictiveness can also be seen as that a theory does not suffer from information loss, in the sense of [23]. One could equally say that future predictiveness is the same as that theory does not suffer information gain, however unlike information loss this is not a popular terminology.

dynamics. In fact this is already true for globally hyperbolic space-times, where if one chooses a time-function that is not Cauchy (but for instance only semi-Cauchy), the time-slicing axiom fails in a sense. That is to say, once one knows the n-point functions of a state in the neighbourhood of an equal time surface, this need not uniquely fix them on the entire space-time.

In the case that our theory has been constructed from a single extended one-particle structure, these predictiveness properties can be one-to-one related with properties of this structure.

Proposition 10. *Given $M = \cup_{j\in J} M_j$ semi-globally hyperbolic and (K, H) an extended one-particle structure, then $\mathcal{A}_{(K,H)}(M)$ is future predictive if and only if for each $j \in J$*

$$K(\mathcal{D}(M_j)) = K(\mathcal{D}(\cup_{j'\geq j} M_{j'})).$$

Proof. Clearly if $K(\mathcal{D}(M_j)) = K(\mathcal{D}(\cup_{j'\geq j} M_{j'}))$, then for any $f \in \mathcal{D}(\cup_{|'\geq|} \mathcal{M}_{|'})$ there exists an $g \in \mathcal{D}(M_j)$ such that $K(f - g) = 0$ and hence

$$\mu(f - g, f - g) = 0.$$

Hence $\hat{\phi}_{(K,H)}(f) = \hat{\phi}_{(K,H)}(g)$ which implies

$$\mathcal{A}_{(K,H)}(M; M_j) \subset \mathcal{A}_{(K,H)}(M; \cup_{j'\geq j} M_{j'}) \subset \mathcal{A}_{(K,H)}(M; M_j).$$

Reversely, given that for each $f \in \mathcal{D}(\cup_{j'\geq j} M_{j'})$ there is a $b \in \mathcal{A}(M; M_j)$ such that

$$b = \hat{\phi}_{(K,H)}(f).$$

Then there are $g_1, ..., g_N \in \mathcal{D}(M_j)$ such that

$$b = \sum_{k_1,...k_N=0}^{M} c_{k_1,...,k_N} (\hat{\phi}(f_1))^{k_1} ... (\hat{\phi}(f_N))^{k_N},$$

and using a similar calculation as the proof of proposition 14, we find that $c_{k_1,...,k_N} = 0$ for $k_1 + ... + k_N > 1$, so we know that (given that b is self-adjoint) there is some $c \in \mathbb{R}$ and $g \in \mathcal{D}(M_j)$ such that

$$b = c + \hat{\phi}_{(K,H)}(g),$$

which implies $\hat{\phi}_{(K,H)}(f - g) = c$, and from the definition of $\mathcal{A}_{(K,H)}$ this can only be so for $c = 0$, which means that

$$\mu(f - g, f - g) = 0$$

and hence $K(f - g) = 0$. Therefore $K(\mathcal{D}(M_j)) = K(\mathcal{D}(\cup_{j'\geq j} M_{j'}))$. □

We have now shown how, given a non-empty set E of extended one-particle structures on semi-globally hyperbolic space-times M, a quantum field theory $\mathcal{A}_E(M)$ can be constructed such that each $(K, H) \in E$ corresponds to a one-particle subspace of a Fock-space representation on $\mathcal{A}_E(M)$. Furthermore we have discussed some aspects of dynamics on these theories. In the next section we will consider some example space-times and show how in various contexts a choice of E can lead to theories with varying degrees of predictiveness.

4 Applications to maximally semi-globally hyperbolic space-times

Here we consider maximally semi-globally hyperbolic space-times. Unless stated otherwise we always define our scalar field algebras with respect to the maximal cover, which means that these theories behave as expected on each causally convex globally hyperbolic neighbourhood. Firstly, we treat space-times that are globally hyperbolic up to a missing point (and hence have a unique completion to a globally hyperbolic space-time), then we will treat space-times with a larger missing region, such that in particular embeddings into globally hyperbolic space-times are highly non-unique, and thirdly we will treat some space-times that cannot be embedded into globally hyperbolic space-times, with particular attention to black hole evaporation space-times.

4.1 Punctured globally hyperbolic space-times

The most elementary class of semi-globally hyperbolic space-time, beyond globally hyperbolic space-times themselves, are space-times that are globally hyperbolic up to a missing point. So in particular, for N globally hyperbolic, and some $p \in N$, the space-time $M = N \setminus \{p\}$ is semi-globally hyperbolic. Note in particular that any Cauchy time-function $T : N \to \mathbb{R}$ restricts to a semi-Cauchy time-function $T\restriction_M$. It is not difficult to see that this space-time is in fact maximally semi-globally hyperbolic, where the maximal cover is given by $M_- = N \setminus \overline{I^+(p)}$ and $M_+ = N \setminus \overline{I^-(p)}$, as illustrated in figure I.4. That this space-time admits a quantum field theory should be clear from the fact that it can be embedded in a globally hyperbolic space-time. Each quasi-free state ω_N on $\mathcal{A}(N)$ defines a one-particle structure (K_N, H_N) on (N, σ_N), which can be restricted to $M_\pm$ to yield a compatible pair of one-particle structures, and so forth. One may however wonder if this is the only interesting quantum field theory one can construct on such a space-time.

In many cases, one wouldn't expect that the absence of a single point in a space-time should leave an imprint on the overall physics. After all, what

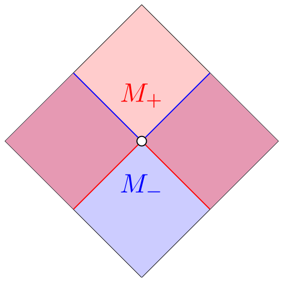

Figure I.4: A punctured globally hyperbolic space-time with maximal cover

kind of physics can be associated with a single point? Certainly in classical field theories, where one is often interested in smooth solutions to equations of motions on smooth space-times, removing a point out of the background will generally not yield any ambiguities of solutions, as long as we restrict ourselves to smooth solutions. In fact, such a result also holds in quantum field theory, where the role of smooth solutions to the equation of motion are now played by (local) Hadamard states, that play an essential role in the definition of higher order observables such as the stress-energy tensor, Wick products and time-ordered products, see [13, 24, 25]. In fact as a consequence of [26, theorem 3.5], we see that given that ω, ω' Hadamard states on a scalar field algebra $\mathcal{A}(M)$, by which we mean that their restriction to $\mathcal{A}(M; M_\pm)$ defines a Hadamard state in the sense of [27], it holds that

$$\omega = \omega' \iff \omega\restriction_{\mathcal{A}(M;M_-)} = \omega'\restriction_{\mathcal{A}(M;M_-)} \iff \omega\restriction_{\mathcal{A}(M;M_+)} = \omega'\restriction_{\mathcal{A}(M;M_+)}.$$

Nevertheless, is some contexts one may also be interested in states that are not Hadamard. This is especially true when one views the missing point in our space-time as some place-holder for singular behaviour, say a point interaction of some kind. In globally hyperbolic space-times it is well known via the propagation of singularities theorem (see [27]) that if a state satisfies the Hadamard condition around some Cauchy surface, it satisfies these conditions on the entire space-time. The same cannot be said for the space-time M introduced here, firstly it does not contain any global Cauchy surface, but at a more fundamental level the missing point can be a source for singular behaviour in distributions. That is to say, suppose that a 2-point function w_2 on the space-time M satisfies the Hadamard conditions on M_-, i.e. following the definitions of [27]

$$WF'(w_2\restriction_{D(M_-)^2}) = \{(x,k;x',k') \in T(M_- \times M_-)\setminus\mathbf{0} : (x,k) \sim (x',k'), k \rhd 0\},$$

then

$$\begin{aligned}WF'(w_2) \subset &\{(x,k;x',k') \in T(M\times M)\setminus \mathbf{0} : (x,k)\sim(x',k'), k \rhd 0\}\\ &\cup \{(x,k;x',k') \in T(M\times M)\setminus \mathbf{0} : TM_+ \ni (x,k)\sim(p,\xi)\\ &\quad \text{or } TM_+ \ni (x',k')\sim(p,\xi) \text{ for some } \xi\in T_pN\}.\end{aligned}$$

Let us give an example. Let (K_-,H_-) and (K_+,H_+) compatible Hadamard one-particle structures inducing faithful Fock space representations on M_- and M_+ respectively, then we can define

$$K'_+ \to \mathcal{D}(M_+) \to H_+ \times \mathbb{C},$$

$$K'_+ f = (K_+ f, G^+(f,p)),$$
$$H'_+ = \overline{K'_+(\mathcal{D}(M_+)) + iK'_+(\mathcal{D}(M_+))},$$

such that for $f,g\in\mathcal{D}(M_+)$

$$\langle K'_+f, K'_+g\rangle'_+ = \langle K_+f, K_+g\rangle_+ + G^+(f,p)G^+(g,p).$$ [8]

By [26, theorem 3.5] we can deduce from the Hadamard property that $K_1(D(M_1\cup M_2)) + iK_1(D(M_1\cup M_2))$ is dense in H_1, therefore

$$(K,H) = (K_-,H_-)\|(K_+,H_+),\ (K',H') = (K_-,H_-)\|(K'_+,H'_+)$$

are the unique extended one-particle structures of these compatible pairs. Since (K,H) corresponds to a quasi-free state on $\mathcal{A}(N)$, we see that

$$\mathcal{A}_{(K,H)}(M) \cong \mathcal{A}(N;M) = \mathcal{A}(N).$$

In particular, $\mathcal{A}_{(K,H)}(M)$ has complete dynamics. However, in the case of (K',H'), the best we can do is find a surjective homomorphism,

$$\mathcal{A}_{(K',H')}(M) \twoheadrightarrow \mathcal{A}(N),$$

with $\hat{\phi}_{(K',H')}(f)\mapsto\hat{\phi}_N(f)$. More specifically

$$\mathcal{A}(N) \cong \mathcal{A}_{(K',H')}(M)\big/\mathcal{I}\ ,$$

with $\mathcal{I}$ the smallest ideal containing all $\hat{\phi}_{(K',G')}(f)$ with

$$f\in\mathcal{D}(M)\cap(\Box - V)\mathcal{D}(N).$$

[8] Note that the new contribution to this inner product has to be real, otherwise it would not respect the pre-symplectic structure on $\mathcal{D}(M_+)$.

It is worth mentioning, that dividing out the ideal $\mathcal{I}$ is not the only way to reduce the theory $\mathcal{A}_{(K',H')}(M)$ to $\mathcal{A}(N)$. For example, given $\lambda_1, \lambda_2 \in \mathbb{R}$, we can define $\mathcal{I}_{\lambda_1,\lambda_2}$ as the smallest ideal such that for any $f \in \mathcal{D}(M) \cap (\Box - V)\mathcal{D}(N)$

$$\hat{\phi}_{(K',G')}(f) + \lambda_1 G^+(f,p) + \lambda_2 G^-(f,p) \in \mathcal{I}_{\lambda_1,\lambda_2}.$$

Even though we have now chosen a different ideal, we see that also in this case we have

$$\mathcal{A}_{(K',H')}(M) \Big/ \mathcal{I}_{\lambda_1,\lambda_2} \cong \mathcal{A}(N).$$

This is not surprising, as one can view the fields $[\hat{\phi}_{(K',H')}(f)]_{\mathcal{I}_{\lambda_1,\lambda_2}}$ as quantizing the classical equation of motion

$$(\Box - V)\phi = -(\lambda_1 + \lambda_2)\delta(.,p)$$

on N. It is well known that quantizing the real scalar field with any external (classical) source always results in the same algebra (see for instance [28]).

These examples illustrate that different choices of extended one-particle structures do not necessarily correspond with different choices of 'boundary conditions', whatever this means for a discrete boundary. In this case it may be sensible to think of a source term at this point p as corresponding to a boundary condition on M. Of course as discussed different choices of these boundary conditions generate the same algebra with the same net-structure, and hence could be though of as equivalent. What we have seen from the theories defined by (K, H) and (K', H') is that they differ in how much 'uncertainty' of such a boundary condition is present in the theory, rather than what actually the boundary condition is. This intimately relates to whether the theory defined has complete dynamics or not.

4.2 Space-times with macroscopic gaps

In the previous subsection we considered space-times that were globally hyperbolic up to one missing point, but of course this can be generalized to larger 'missing regions', for instance a space-like disk. Let us give a slightly more abstract description of what kind of space-time we consider in this section.

Let $M = M_- \cup M_+$ maximally semi-globally hyperbolic with $T : M \to \mathbb{R}$ a semi-Cauchy time-function such that $T^{-1}(\{0\})$ is a smooth Cauchy surface of $M_- \cap M_+$, and $\Sigma_{\pm t} = T^{-1}(\{\pm t\})$ a Cauchy surface of $M_\pm$ for each $t > 0$. So far this is nothing new, but now we assume that

$$\Sigma_{-t} \cong \Sigma_t,$$

and that M can be isometrically embedded in some N such that

$$\Sigma_{\pm} = \lim_{t \downarrow 0} \Sigma_{\pm t},$$

which should be interpreted as the sets of all limits of sequences in $\prod_{n\in\mathbb{N}} \Sigma_{\pm\frac{1}{n}}$, are also smooth Cauchy surfaces of $\mathcal{D}(M_{\pm}) \subset N$. Furthermore we require that $\Sigma_0 = \Sigma_+ \cap \Sigma_-$ and that there is a diffeomorphism

$$d : \Sigma_- \to \Sigma_+,$$

that leaves Σ_0 invariant.

Note that nowhere we have explicitly required that the ambient space-time N is in itself globally hyperbolic, though in practice we can often choose it to be that way. In this case such an embedding can be used to directly define a quantum field theory on M via $\tilde{\mathcal{A}}(M) = \mathcal{A}(N; M)$ which, due to the fact that N is by no means uniquely defined, already shows that there are a lot of different free scalar quantum field theories that can be defined on M. However, there is another way one can construct such quantum field theories, which do not make direct use of N, but only use the surfaces $\Sigma_{\pm}$ and the diffeomorphism d.

Suppose we have a one-particle structure (K_-, H) on M_-. Consider a test-function $f_+ \in \mathcal{D}(M_+)$, we know that $\Delta_{M_+}(f_+) \in \mathcal{E}(M_+)$ induces a function $\varphi_+(f_+) = \Delta_{M_+}(f_+)\restriction_{\Sigma_+} \in \mathcal{D}(\Sigma_+)$ and a smooth distribution $\pi_+(f_+) \in \mathcal{E}'(\Sigma_+)$ given by

$$(\pi_+(f_+), u) = \int_{\Sigma_+} dA(u \nabla_{\mathbf{n}} \Delta_{M_+}(f_+)).$$

We can now define $\varphi_-(f_+) = \varphi_+(f_+) \circ d \in \mathcal{D}(\Sigma_+)$ and $\pi_-(f_+) \in \mathcal{E}'(\Sigma_-)$ via

$$(\pi_-(f_+), u) = (\pi_+(f_+), u \circ d^{-1}).$$

It is not hard to see that $\pi_-(f_+)$ has a smooth compact integration kernel and hence via theorem 11 $\varphi_-(f_+)$ and $\pi_-(f_+)$ define a unique spatially compact solution to the Klein-Gordon equation $\Delta_-(f_+) \in \mathcal{E}(M_-)$. We can now find an $f'_+ \in \mathcal{D}(M_-)$ such that $\Delta_{M_-}(f'_+) = \Delta_-(f_+)$, which we use to define $K_+ : \mathcal{D}(M_+) \to H$ via $K_+(f_+) = K_-(f'_+)$. Here we note that $K_-(f'_+)$ is independent of the choice of $f'_+ \in \Delta^{-1}_{M_-}(\{\Delta_-(f_+)\})$. One can show that (K_+, H) defines a one-particle structure on M_+. After all for $f_+, g_+ \in \mathcal{D}(M_+)$ we have

$$\begin{aligned}
2Im(\langle K_+ f_+, K_+ g_+ \rangle) =& 2Im(\langle K_- f'_+, K_- g'_+ \rangle) \\
=& \sigma_{M_-}(f'_+, g'_+) \\
=& (\pi_-(g_+), \varphi_-(f_+)) - (\pi_-(g_-), \varphi_-(f_-)) \\
=& (\pi_+(g_+), \varphi_+(f_+)) - (\pi_+(g_-), \varphi_+(f_-)) \\
=& \sigma_{M_+}(f_+, g_+),
\end{aligned}$$

furthermore $(K_+ \circ (\Box - V))(f_+) = K_-(0) = 0$, and since d is invertible $K_+(\mathcal{D}(M_+)) = K_-(\mathcal{D}(M_-))$. From the fact that d leaves Σ_0 invariant, we also see that

$$K_- \restriction_{\mathcal{D}(M_- \cap M_+)} = K_+ \restriction_{\mathcal{D}(M_- \cap M_+)},$$

which implies in particular that (K_-, H) and (K_+, H) form a compatible pair.

In principle we can now define $(\tilde{K}, H) = (K_-, H) \| (K_+, H)$. However in general this one-particle structure does not lead to a theory with well-posed global dynamics. In this particular case, we can define $K : \mathcal{D}(M) \to H$ more directly, where for $f = f_+ + f_-$ with $f_\pm \in \mathcal{D}(M_\pm)$ we set

$$Kf = K_+ f_+ + K_- f_-.$$

The quantum field theory $\mathcal{A}_{(K,H)}(M)$ that this extended one-particle structure

$$(K, H)$$

defines actually only depends on the choice of d and not on (K_-, H). In fact we can give an alternative construction of this algebra that bypasses the use of these extended one-particle structures. We first extend the maps π_- and φ_- to $\mathcal{D}(M)$ in the natural way, i.e. such that for $f_- \in \mathcal{D}(M_-)$ we have $\varphi_-(f_-) = \Delta_{M_-}(f_-)\restriction_{\Sigma_-}$ and so forth. We then see that

$$\mathcal{A}_{(K,H)}(M) = \mathcal{A}_d(M) = \mathcal{B}(M)/\mathcal{J}_d\ ,$$

with $\mathcal{J}_d$ the smallest ideal such that for each $f, g \in \mathcal{D}(M)$ we have that

$$[\hat{\psi}(f), \hat{\psi}(g)] - i((\pi_-(g), \varphi_-(f)) - (\pi_-(g), \varphi_-(f))) \in \mathcal{J}_d,$$

and given that $\varphi_-(f) = 0$ and $\pi_-(f) = 0$ we have

$$\hat{\psi}(f) \in \mathcal{J}_d.$$

Note also that this theory has complete dynamics, which is due to the fact that d is a diffeomorphism. Nevertheless, as we will see in section 5.1, the construction above can be generalized to the case where d is a manifold embedding instead of a diffeomorphism, but in this case these theories will generally not be either past or future predictive.

4.3 Black hole evaporation space-times

The examples we have considered so far could mostly be embedded in globally hyperbolic space-times. While these examples did allow us to play around with the constructions outlined in section 3.1, these space-times itself, or rather the quantum field theories on these space-times that deviate from the theories on their embedding into globally hyperbolic space-times, are of limited physical interest. We now focus our attention on a class of maximally semi-globally hyperbolic space-time that have played a relevant role in the physics literature over the past decades, namely the 'black hole evaporation' space-times. First introduced in [11], (spherically symmetric) black hole evaporation space-times are characterized by their Penrose diagram, drawn in figure I.3, and supposedly model a black hole that loses energy due to Hawking radiation (a quantum field theoretical phenomenon which was also first discussed in [11]) and are thought to shrink into nothingness due to the semi-classical back-reaction of this radiation on the space-time metric. It should be noted that no explicit semi-classical solution to general relativity coupled to a scalar quantum field theory (via the semi-classical Einstein equations) is known that models formation and evaporation of a black hole, nor is it known if such solutions actually exist. Nevertheless the suggestion that such solutions may exist in this framework has lead to significant controversy, which often goes under the name of the information loss paradox [29, 30]. Covering this discussion goes beyond the scope of this text. Nevertheless we do reiterate the point of view pushed most notably in [23] that, as already alluded to when we wrote down definition 11, from the perspective of quantum field theory on curved space-time, information loss in itself is not at odds with any theoretical foundations. Quantum field theories on semi-globally hyperbolic space-times need not have complete dynamics (with respect to some semi-Cauchy time-function). The time-slicing property is only assumed to hold with respect to Cauchy surfaces. Since black hole evaporation space-times are not globally hyperbolic, information loss (or even information gain) is, at the level of semi-classical physics, not at all problematic. Of course when one believes that semi-classical physics approximates an underlying quantum gravity theory that by assumptions does not admit information loss, one would either need to explain how information losing processes can emerge in the semi-classical limit, or argue that black hole evaporation does not occur in the way that one would expect based on semi-classical arguments.

So having established that in principle a theory admitting information loss on black hole evaporation space-times is not against any foundations of quantum field theory, a question that should be addressed is whether or not one can actually construct such a theory in the first place. Using the constructions that we have considered in this paper, we argue that black hole evaporation space-times do admit linear scalar quantum field theories, however we will see that this leads to a problem that is arguably more problematic than information loss (at least from a semi-classical point of view), as it is unclear if the resulting quantum field theory admits any (physically reasonable) states.

Given that M is a black hole evaporation space-time, the construction of $\mathcal{A}(M)$ is based on the observation that M can be approximated by space-times with macroscopic gaps as discussed in section 4.2. That is to say, the maximally globally hyperbolic space-time $M = M_+ \cup M_-$ contains a nested sequence $M^{(n)} = M_+^{(n)} \cup M_-^{(n)}$ in the class of space-times introduced in section 4.2, with

$$M_\pm^n \subset M_\pm^{n+1} \subset M_\pm \subset M,$$

such that

$$M = \bigcup_n M^{(n)}, \text{ and } D(M_\pm^{(n)}) = M_\pm.$$

As we've seen in section 4.2 we can always construct an extended one-particle structure on $M^{(n)}$, say $(K^{(n)}, H^{(n)})$, which we could even choose such that $\mathcal{A}_{(K^{(n)},H^{(n)})}(M^{(n)})$ has complete dynamics.

Now choose $E^{(n)}$ to be the set of all (unitary inequivalent) extended two-point functions on $M^{(n)}$. Note that there are unique injective maps $\iota_n : E^{(n+1)} \to E^{(n)}$ such that, given $(K^{(n)}, H^{(n)}) = \iota_n((K^{(n+1)}, H^{(n+1)}))$, for each $f, g \in \mathcal{D}(M^{(n)}) \subset \mathcal{D}(M^{(n+1)})$ we have

$$\langle K^{(n)} f, K^{(n)} g\rangle^{(n)} = \langle K^{(n+1)} f, K^{(n+1)} g\rangle^{(n+1)}.$$

That this map is injective and unique follows from the fact that for each $f \in \mathcal{D}(M^{(n+1)})$ there is (using the wave equation) a function $g \in \mathcal{D}(M^{(n)})$ such that $K^{(n+1)} f = K^{(n+1)} g$. Therefore $K^{(n)}$ uniquely determines $K^{(n+1)}$ (up to a unitary map). By the same argument we have that $H^{(n)} \cong H^{(n+1)}$. This means that there are natural embeddings

$$\mathfrak{H}_{E^{(n+1)}} \subset \mathfrak{H}_{E^{(n)}}$$

of the Hilbert spaces as given in definition 10, which means in particular that we can define a Hilbert space projector $p^{(n)} : \mathfrak{H}_{E^{(n)}} \to \mathfrak{H}_{E^{(n+1)}}$.

Shifting our attention to the algebras $\mathcal{A}_{E^{(n)}}(M^{(n)})$, we note that we can define surjective maps

$$\kappa^{(n)} : \mathcal{A}_{E^{(n)}}(M^{(n)}) \twoheadrightarrow \mathcal{A}_{E^{(n+1)}}(M^{(n)}),$$

given by $\hat{\phi}_{E^{(n)}}(f) \mapsto p^{(n)} \hat{\phi}_{E^{(n)}}(f) p^{(n)}$. That this map is surjective again follows from that the $\hat{\phi}_{E^{(n)}}$'s satisfy the wave equation. This allows us to define a nested sequence of ideals $\mathcal{I}^{(n)} \subset \mathcal{A}_{E^{(1)}}(M^{(1)})$ defined by

$$\mathcal{I}^{(n)} = \ker(\kappa^{(n-1)} \circ \ldots \circ \kappa^{(1)}).$$

This yields

$$\mathcal{I}^{(n)} \subset \mathcal{I}^{(n+1)}, \text{ and } \mathcal{A}_{E^{(1)}}(M^{(1)})\big/\mathcal{I}^{(n)} \cong \mathcal{A}_{E^{(n)}}(M^{(n)}).$$

We now define

$$\mathcal{A}(M) = \mathcal{A}_{E^{(1)}}(M^{(1)})\Big/\left(\bigcup_n \mathcal{I}^{(n)}\right).$$

where for $f \in \mathcal{D}(M)$ one defines $\hat{\phi}(f) = [\hat{\phi}_{E^{(1)}}(f')]_{\bigcup_n \mathcal{I}^{(n)}}$ for $f' \in \mathcal{D}(M^{(1)})$ with $f - f' \in (\Box - V)\mathcal{D}(M)$. This allows $\mathcal{A}(M)$ to be given a net structure in the usual way, where we can see that for each $U \subset M$ causally convex globally hyperbolic

$$\mathcal{A}(M; U) \cong \mathcal{A}(U).$$

From here it is clear that $\mathcal{A}(M)$ is a linear scalar quantum field theory in the sense of definition 5.

Until now all the theories that we constructed admitted states by design, we first constructed a state (or rather one-particle structure) that our theory should admit and built the algebra from there. The construction above does not start from a state on $\mathcal{A}(M)$, but rather from a sequence of what one could arguably call ‘approximate states’, in the sense that these states are defined everywhere on the space-time up to some small neighbourhood of the black hole singularity, which can be made arbitrarily small. In other words, if one allows the physics to deviate (in an a priori unspecified way) from the semi-classical model in an arbitrarily small neighbourhood of the singularity, then one could hope that one of these ‘approximate states’ defines an algebra that describes the physics away from the singularity in a sufficiently accurate way, perhaps even yielding a theory that has complete dynamics. This idea is in itself nothing new, after all one expects that near the singularity, where curvature of the space-time blows up, that the semi-classical approximation breaks down and one needs an underlying theory of quantum gravity to accurately describe the situation. For this reason researchers working in several quantum gravity communities have proposed various quantum gravity mechanisms that could play a role in this regime. A recent example of this is the black hole to white hole tunnelling mechanism that has been studied in [31]. Such a mechanism would indeed yield a space-time that, outside this transition region, looks exactly like one of these $M^{(n)}$'s, where the precise choice of $(K^{(n)}, H^{(n)}) \in E^{(n)}$ that can be used to define the quantum field theory on $M^{(n)}$ should somehow follow from the underlying quantum gravity theory.

The question that remains, is whether $\mathcal{A}(M)$ admits any states at all. This is an open question as far as the author is concerned. From the discussion following definition 5, one can construct a Weyl-like algebra $\mathfrak{A}(M)$ associated with $\mathcal{A}(M)$ which does admit states. However whether any of these states can be extended to $\mathcal{A}(M)$, i.e. whether these states define n-point functions, should be further analysed. One could hope that there exists some unit vector in $\bigcap_n \mathfrak{H}_{E^{(n)}}$, which if it existed does define a state on $\mathcal{A}(M)$, but unfortunately the set of unit vectors in $\mathfrak{H}_{E^{(n)}}$ is not compact, and only its convex hull is weakly compact (by the Banach-Alaoglu theorem, see [32]), hence Cantor's intersection theorem does not yield any non-zero elements in $\bigcap_n \mathfrak{H}_{E^{(n)}}$. Therefore, as far as we can tell the only way to decide whether $\mathcal{A}(M)$ admits any physically reasonable states would be an explicit calculation. This calls for further investigation.

5 Some applications to non-maximally semi-globally hyperbolic space-times

In the previous section we discussed some constructions of quantum field theories on maximally semi-globally hyperbolic space-times. Due to the nature of these space-times, the theories constructed automatically reduce to the standard theory on globally hyperbolic space-times on each globally hyperbolic causally convex region. However in some cases we would like to construct quantum field theories on more general semi-globally hyperbolic space-times. In this section we give two examples of such a construction.

5.1 Topology changing space-times

The first example that we will treat is a topology changing space-times. Topology change has mostly been considered in the context of creating wormholes, see for instance [33]. As mentioned in this paper, topology change in space-times without naked singularities is only possible when the space-time either contains closed time-like curves or is not time-orientable (see theorem 2 in [34]). However, our class of semi-globally hyperbolic space-times do allow for naked singularities and hence one may be able to construct worm-hole space-times that do fall in this class. Another example where topology change plays a role are in so-called branching space-times (see for instance [35]), which are meant to model indeterminism.

While we do not explicitly consider a branching space-time nor a wormhole space-time, here we merely give a proof of principle that quantum field theories can be constructed on at least some topology changing space-time. In particular, we consider a semi-globally hyperbolic space-time $M = M_- \cup M_+$ with M_+ having Cauchy surfaces $\Sigma_+ \cong \mathbb{R}^3$ and M_- having Cauchy surfaces

$\Sigma_- \cong \mathbb{R}^2 \times \mathbb{S}$. We assume these space-times have a flat geometry and we have drawn a Penrose diagram of the space-time (having reduced the $\mathbb{R}^2$ symmetry) in figure I.5.

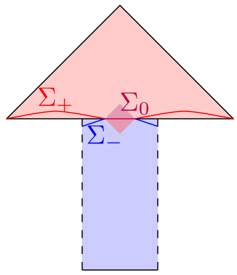

Figure I.5: Penrose diagram of the topology changing space-time M with two spatial directions of translational symmetry suppressed

As one can see in this Penrose diagram, we are nearly in the same situation as in section 4.2, where $\Sigma_0 = \Sigma_- \cap \Sigma_+$ is a Cauchy surface of $M_- \cap M_+$, except for the fact that there is no diffeomorphism between Σ_- and Σ_+, but we can find some submanifold $\Sigma_0 \subset U \subset \Sigma_-$ such that $d : U \to \Sigma_+$ is a diffeomorphism leaving Σ_0 invariant. This allows us to define for each $f_+ \in \mathcal{D}(M_+)$ an $\varphi_-(f_+) \in \mathcal{D}(U) \subset \mathcal{D}(\Sigma_-)$ and $\pi_-(f_+) \in \mathcal{E}'(U) \subset \mathcal{E}'(\Sigma_-)$ with smooth integral kernel which we can use to define an extended one-particle structure (K, H) from any one-particle structure (K_-, H) on M_-. This allows us to construct a linear scalar quantum field theory on $\mathcal{A}_d(M)$ in exactly the same way as for the macroscopic gap space-times, however with the notable difference that $\mathcal{A}_d(M)$ has no complete dynamics, while it is not past predictive. However it future predictive, as we see that $\mathcal{A}_d(M; M_+) = \mathcal{A}_d(M)$.

5.2 Approximating time-like boundaries

As mentioned in the introduction, one class of non-globally hyperbolic space-times on which quantum field theory has already been well-studied in [4], are (certain) space-times with time-like boundaries. While these space-times are not semi-globally hyperbolic, we can still use our construction to make contact with quantum field theories on these backgrounds.

The class of space-times that we consider here are *globally hyperbolic space-times with time-like boundaries* (as defined in [6]). These space-times notably still satisfy a version of Geroch's splitting theorem. In particular, let M the bulk of a globally hyperbolic space-time with time-like boundary $\overline{M}$, then there is a time-function $t : M \to \mathbb{R}$ such that each level surface $t = T$ is an acausal hypersurfaces Σ_T. In particular $\overline{\Sigma_T}$ is Cauchy in $\overline{M} \cong \mathbb{R} \times \overline{\Sigma_T}$. We claim that we can approximate this space-time by semi-globally hyperbolic space-times.

We define

$$M^{(n)} = \bigcup_{k=-\infty}^{\infty} \bigcup_{l=0}^{2^n-1} D\left(\Sigma_{k+\frac{l}{2^n}}\right) \subset M,$$

which clearly yields a nested sequence

$$M^{(n)} \subset M^{(n+1)}.$$

Furthermore for each $x \in M$ with $T(x) = t$, we can define $t' = \inf(T^{-1}(J^+(x) \cap \partial M)) > t$. Choosing k, l, m such that $t < k + \frac{l}{2^n} < t'$, we see that each inextendible causal curve through x must cross $\Sigma_{k+\frac{l}{2^n}}$ and hence $x \in M^{(n)}$. We conclude that

$$\bigcup_{n \in \mathbb{N}} M_n = M.$$

Now in principle we could consider $E^{(n)}$ again as the set of all (unitarily inequivalent) extended one-particle structures on $M^{(n)}$. Similarly to the case of the black hole evaporation space-time, this yields a chain of surjective *-isomorphisms

$$\kappa^{(n)} : \mathcal{A}_{E^{(n)}}(M^{(n)}) \twoheadrightarrow \mathcal{A}_{E^{(n+1)}}(M^{(n+1)}),$$

and allow us to define

$$\mathcal{A}(M) = \mathcal{A}_{E^{(1)}}(M^{(1)}) \Big/ \bigcup_n \ker(\kappa^{(n)} \circ \ldots \circ \kappa^{(1)}) \,.$$

Here the quasi-free states $\mathcal{A}(M)$ can be characterized by the one-particle structures $(K, H) \in E$ on M.[9]

The construction outlined above is actually inequivalent to the universal extension algebra as constructed in [4]. Firstly $\mathcal{A}(M)$ is constructed such that there exist generators $\{\hat{\phi}(f) : f \in \mathcal{D}(M)\} \in \mathcal{A}(M)$, where $[\hat{\phi}(f), \hat{\phi}(g)]$ is in the center of $\mathcal{A}(M)$. This is not true for the universal extension algebra. Another difference is that while the universal extension algebra is constructed to reduce to the standard quantum field algebra on each globally hyperbolic causally convex $U \subset M$, in the case of $\mathcal{A}(M)$ this is only satisfied when $U \subset D(\Sigma_T)$ for some $T \in \mathbb{R}$. Here we see that the fact that definition 5 depends on the choice of a semi-Cauchy time-function can actually be a strength instead of a weakness. The construction of [4] as well as the construction above can both

[9] Note that, if non-empty, E can be identified with the inverse limit $\lim_{\leftarrow} E^{(n)}$.

be used for implementing local boundary conditions such as the Dirichlet condition (see [2]), however if one wants to implement non-local conditions, such as periodic boundary conditions, the former construction can no longer be used. In the case of periodic boundary conditions, where we assume our space-time M to have two diffeomorphic disjoint time-like boundaries $\partial M = B_1 \cup B_2$, an identification of these boundaries $\iota : B_1 \to B_2$ induces a new effective causal structure $\leq_\iota$ on the space-time. In general, a causally convex $U \subset M$ need not be causally convex with respect to $\leq_\iota$, which is why once cannot expect a theory respecting these boundary conditions to reduce to the standard theory on U and hence the construction of [4] is not suitable. However, if one can find a time-function $t : M \to \mathbb{R}$ that is compatible with $\leq_\iota$, i.e. for each $x \leq_\iota x'$ we have $t(x) \leq t(x')$, the construction outlined above is sufficiently versatile to be compatible with these boundary conditions.

However, both constructions generally do not have complete dynamics. Of course in our construction we did not make reference to a particular choice of boundary conditions, so first these will need to actually be imposed by dividing out a further ideal from $\mathcal{A}(M)$. As in [4], we can construct such an ideal $\mathcal{I}_{G_\pm}$ from an adjoint pair of retarded and advanced propagators (G_+, G_-) satisfying the desired boundary conditions. Here it should be noted that for this algebra $\mathcal{A}_{G_\pm}(M) = \mathcal{A}(M) \Big/ \mathcal{I}_{G_\pm}$ to admit any states, we need to make sure that there exists an extended one-particle structure $(K, H) \in E$ such that

$$\int_M dV f (G_+ - G_-) g = 2 Im \left(\langle K f, K g \rangle \right).$$

As was also concluded in [4], if one compares the resulting algebra to explicit constructions of quantum field theories, such as made in [2], one finds that the resulting algebra $\mathcal{A}_{G_\pm}(M)$ does not capture all relevant degrees of freedom, only those that can be localized in the interior. This has as a consequence that the dynamics on $\mathcal{A}_{G_\pm}(M)$ is still not complete. In general, one needs to also consider boundary degrees of freedom to construct a complete theory on space-times with time-like boundaries.

6 Concluding remarks

We have seen that one can construct linear scalar quantum field theories on various semi-globally hyperbolic space-times. Using the constructions of section 3.1 we saw that on any semi-globally hyperbolic space-time we can define a scalar field algebra that admits states if and only if one could define a compatible chain of one-particle structures on that space-time. Nevertheless we have also seen that in some cases, such as in the case of the evaporating black hole space-time, one can construct scalar field algebras, but it is a priori unclear if such an algebra admits any state. On the one hand this is very much in the spirit of algebraic quantum field theory, where one aims to disentangle purely algebraic considerations and questions concerning states and representations. Arguably, the observation that on non-globally hyperbolic space-times, such as the black hole evaporation space-time, constructing an algebra is not so problematic, but that the problems mainly arise when one wants to find physically reasonable states, fits very well in this tradition. On the other hand, the methods that we used to arrive at this construction explicitly made use of one-particle structures and representations of the to be constructed (sub)algebras. This means that, unlike for the well-established construction of linear scalar quantum field theory on globally hyperbolic space-times, the separation between algebras and representations has not been made very cleanly in this work. Whether this is a shortcoming of our constructions, or rather hints at the fact that the conceptual separation of algebras and their representation is a luxury that one cannot always afford, is, as far as the author of this paper is concerned, open for debate.

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Appendix A. Recalling a construction on globally hyperbolic space-times

In order to construct quantum field theories on semi-globally hyperbolic space-times, we need to recall some facts about the linear scalar (quantum) field on globally hyperbolic space-times. On these space-time (1) has a well posed initial value problem, as proven for instance in [37].

Theorem 11. *Let M globally hyperbolic, Σ a smooth acausal Cauchy surface, $\mathbf{n} \in \mathfrak{X}(M)$ normal to Σ, $f \in \mathcal{D}(M)$ and $\varphi, \pi \in \mathcal{D}(\Sigma)$. Then there is a unique*

$F \in \mathcal{E}(M)$ such that

$$(\Box - V)F = f,\ F\restriction_\Sigma = \varphi,\ \nabla_\mathbf{n} F\restriction_\Sigma = \pi.$$

Furthermore $F \in J(\mathrm{supp}(f) \cup \mathrm{supp}(\varphi) \cup \mathrm{supp}(\pi))$.[10]

It is this (classical) result that motivates the restriction to globally hyperbolic space-times when constructing a quantum field theory. In part, this is related to the following consequence of the theorem above.

Corollary. *Let M globally hyperbolic, there are two linear maps*

$$G_\pm : \mathcal{D}(M) \to \mathcal{E}(M),$$

referred to as the advanced *and* retarded propagator*, uniquely defined by*

$$(\Box - V)G_\pm(f) = f,\ \mathrm{supp}(G_\pm(f)) \subset J^\pm(\mathrm{sup}(f)).$$

Using these propagators, one can make the following definition:

Definition 12. *The* causal propagator

$$\Delta : \mathcal{D}(M) \to \mathcal{E}(M),$$

is defined as

$$\Delta(f) = G_+(f) - G_-(f).$$

This causal propagator plays a key role in the construction of the linear scalar quantum field, in particular in fixing the commutator relations of the algebra of field observables. It has the following properties, as proven in [13].

Theorem 12. *Let M globally hyperbolic, Σ a smooth Cauchy surface, $\mathbf{n} \in \mathfrak{X}(M)$ normal to Σ. Then*

1. *The range of the causal propagator $\mathcal{S}_{s.c.}(M) := \Delta(\mathcal{D}(M))$ is the set of all spatially compact solutions to the equation of motion, i.e. $F \in \mathcal{S}_{s.c}(M)$ iff*

$$(\Box - V)F = 0,\ F\restriction_\Sigma, \nabla_\mathbf{n} F\restriction_\Sigma \in \mathcal{D}(\Sigma).$$

[10] To clarify some (standard) notation, $\mathfrak{X}(M)$ is the set of real vectorfields on M, i.e. smooth sections of the tangent bundle TM, $\mathcal{D}(M)$ is the vectorspace of smooth real scalar functions on M with compact support (usually referred to as test functions and given an appropriate topology which we do not consider here), $\mathcal{E}(M)$ is the space of arbitrary real smooth functions on M and $J(U)$ is the set of all points in M connected to some point $p \in U \subset M$ via a causal curve.

2. The kernel of Δ is the linear subspace $(\Box - V)\mathcal{D}(M) \subset \mathcal{D}(M)$.[11]

3. For $f \in \mathcal{D}(M)$ and $F \in \mathcal{E}(M)$ with $(\Box - V)F = 0$, we have

$$\int_M dV fF = \int_\Sigma dA(\Delta(f)\nabla_{\mathbf{n}}F - F\nabla_{\mathbf{n}}\Delta(f))\restriction_\Sigma.$$

4. Defining for $f, g \in \mathcal{D}(M)$

$$\sigma_M(f, g) = \int_M dV f\Delta(g),$$

we have

$$\sigma_M(f, g) = \int_\Sigma dA(\Delta(f)\nabla_{\mathbf{n}}\Delta(g) - \Delta(g)\nabla_{\mathbf{n}}\Delta(f))\restriction_\Sigma.$$

As a consequence σ_M defines a symplectic form on $\frac{\mathcal{D}(M)}{(\Box-V)\mathcal{D}(M)}$, i.e. a non-degenerate anti-symmetric bi-linear map.

The symplectic space of classical solutions given above forms the basis for the construction of the (real) scalar quantum field. This construction, which generalizes the more familiar canonical quantization of the scalar field on Minkowski space, can be traced back to [38], albeit in a Weyl algebra formulation. Here we will give a formulation more similar to the construction as in [1, Chapter 3].

Given a certain potential, the algebra of linear observables on M is defined as the so-called CCR algebra of the symplectic space

$$\left(\frac{\mathcal{D}(M)}{(\Box - V)\mathcal{D}(M)}, \sigma_M\right).$$

Informally, this is given as the unital *-algebra $\mathcal{A}(M)$ generated by elements

$$\{\hat{\phi}(f) : f \in \mathcal{D}(M)\},$$

subject to the following relations:

$$\begin{aligned} \forall f, g \in \mathcal{D}(M), a \in \mathbb{R} : \hat{\phi}(af + g) &= a\hat{\phi}(f) + \hat{\phi}(g), \\ \forall f \in \mathcal{D}(M) : \hat{\phi}(f)^* &= \hat{\phi}(f), \\ \forall f, g \in \mathcal{D}(M) : [\hat{\phi}(f), \hat{\phi}(g)] &= i\sigma_M(f, g)\mathbb{1}, \\ \forall f \in \mathcal{D}(M) : \hat{\phi}((\Box - V)f) &= 0. \end{aligned}$$

This is made precise in the following definition, which for future purposes constructs $\mathcal{A}(M)$ in two steps.

[11] Combining point 1 and 2, we see that Δ defines a linear isomorphism between $\frac{\mathcal{D}(M)}{(\Box-V)\mathcal{D}(M)}$ and $\mathcal{S}_{s.c}(M)$.

Definition 13. *For a (not necessarily globally hyperbolic) space-time M, we define the* pre-field algebra of real linear scalar observables $\mathcal{B}(M)$ *in the following way. Let $\langle\mathcal{D}(M)\rangle$ the unital free *-algebra over $\mathbb{C}$ generated by $\mathcal{D}(M)$.*[12] *Define $\mathcal{I} \subset \langle\mathcal{D}(M)\rangle$ as the smallest ideal such that for each $f, g \in \mathcal{D}(M)$ and $a \in \mathbb{C}$ we have*

$$\langle af + g\rangle - a\langle f\rangle - \langle g\rangle \in \mathcal{I},$$

$$\langle f\rangle - \langle f\rangle^* \in \mathcal{I}.$$

Define

$$\mathcal{B}(M) := \langle\mathcal{D}(M)\rangle/\mathcal{I}\ ,$$

and denote for $f \in \mathcal{D}(M)$

$$\hat{\psi}(f) := [\langle f\rangle]_{\mathcal{I}}.$$

For M globally hyperbolic, we can define the linear scalar quantum field algebra $\mathcal{A}(M)$. *Let $\mathcal{J} \subset \mathcal{B}(M)$ be the smallest ideal such that for each $f, g \in \mathcal{D}(M)$*

$$[\hat{\psi}(f), \hat{\psi}(g)] - i\sigma_M(f, g)\mathbb{1} \in \mathcal{J},$$

and for $f \in \mathcal{D}(M)$ such that for all $g \in \mathcal{D}(M)$

$$\sigma_M(f, g) = 0,$$

we also have

$$\psi(f) \in \mathcal{J}.$$

We now set

$$\mathcal{A}(M) := \mathcal{B}(M)/\mathcal{J}\ .$$

For each $f \in \mathcal{D}(M)$ denote

$$\hat{\phi}(f) := [\hat{\psi}(f)]_{\mathcal{J}} \in \mathcal{A}(M).$$

*Both $\mathcal{B}(M)$ and (for M globally hyperbolic) $\mathcal{A}(M)$ are given a netstructure where for $U \subset M$ open, $\mathcal{B}(M, U) \subset \mathcal{B}(M)$ the smallest unital *-subalgebra such that for each $f \in \mathcal{D}(M)$ with supp$(f) \subset U$ we have $\psi(f) \in \mathcal{B}(M; U)$, from which can we define for M globally hyperbolic*

$$\mathcal{A}(M; U) = [\mathcal{B}(M; U)]_{\mathcal{J}}.$$

[12] The unital free *-algebra can be seen as the algebra of polynomials over $\mathbb{C}$ with the noncommuting variables $\langle f\rangle$ and $\langle f\rangle^*$ for $f \in \mathcal{D}(M)$.

Observe that the pre-field algebra contains no information on dynamics whatsoever. Both the dynamics of the field and commutation relations are implemented by the quotient $\mathcal{A}(M) := \mathcal{B}(M)/\mathcal{J}$., where we should note that if $\sigma_M(f,g) = 0$ for all $g \in \mathcal{D}(M)$, this is equivalent to $\Delta f = 0$ and hence also to $f \in (\Box - V)\mathcal{D}(M)$, as we saw in theorem 12.

While there are many equivalent ways of defining this algebra of observables, just as there are many ways of describing effectively the same symplectic space of classical solutions, the construction above lends itself very well to the interpretation of the linear observables as being generated by an 'operator valued distribution' with integral kernel $\hat{\phi}(x)$ satisfying the equation of motion.

It should be noted that the net structure $\mathcal{A}(M;\cdot)$ (i.e. a net of *-algebra's indexed by open subsets $U \subset M$ satisfying $\mathcal{A}(M;U) \subset \mathcal{A}(M;V)$ whenever $U \subset V$), has the following convenient properties, as shown to hold in [1, Chapter 3].

Theorem 13. *Let M globally hyperbolic, $U, V \subset M$. Then*

1. *If U and V not causally related, i.e. there is no causal curve connecting U and V, then*
$$[\mathcal{A}(M;U), \mathcal{A}(M;V)] = \{0\}.$$
This property is referred to as Einstein causality*.*

2. *If there is a Cauchy surface $\Sigma \subset M$ such that $\Sigma \subset U$, then*
$$\mathcal{A}(M;U) = \mathcal{A}(M).$$
This is known as the time-slicing property*.*

3. *If U causally convex (and as a result, globally hyperbolic in itself, see [39, prop. 6.6.2]), then there is a *-isomorphism*
$$\iota : \mathcal{A}(U) \to \mathcal{A}(M;U),$$
where $\iota(\hat{\phi}_U(f)) = \hat{\phi}_M(f)$.

Historically, these net structures of *-algebras were used as the basis for an axiomatic framework to formalize the notion of quantum field theories on Minkowski space-time, see in particular the Haag-Kastler nets as introduced in [40]. It was this algebraic approach to quantum field theory that formed the basis for Dimock's generalization of the linear scalar field to arbitrary globally hyperbolic space-times in [38]. In [17] and references therein it was then recognized that the mathematical structures of nets of algebras on globally hyperbolic space-times could be further generalized into the framework of category theory. Here it is noted that, as a result of point 3 of theorem 13, $\mathcal{A}$ can be seen as a functor from the category of globally hyperbolic space-times (referred to as **Loc**), where morphisms are given by causally convex embeddings, to the category of *-algebras **Alg**, where the morphisms are given by *-homomorphisms. This forms the basis of a general axiomatic framework to describe covariant quantum field theories on arbitrary globally hyperbolic space-times.

Of course where there is a *-algebra associated with a physical theory there is a notion of states. We recall the definition.

Definition 14. *Let $\mathcal{A}$ be a unital *-algebra. A* state *is a linear map*

$$\omega : \mathcal{A} \to \mathbb{C},$$

such that $\omega(1) = 1$ and for each $a \in \mathcal{A}$ we have $\omega(aa^*) \geq 0$.

For a globally hyperbolic space-time M, states on the algebra $\mathcal{A}(M)$ are uniquely characterized by their n-point functions

$$w_n : \mathcal{D}(M)^n \to \mathbb{C},$$

where $w_n(f_1, ..., f_n) = \omega(\hat{\phi}(f_1)...\hat{\phi}(f_n))$. We recall an important class of states for the linear scalar fields.

Definition 15. *A state ω on $\mathcal{A}(M)$ is called quasi-free if there is a positive semi-definite symmetric bilinear form (i.e. a real pre-inner product) $\mu : \mathcal{D}(M)^2 \to \mathbb{R}$ satisfying*

$$|\sigma_M(f, g)|^2 \leq 4\mu(f, f)\mu(g, g),$$

such that for each $f \in \mathcal{D}(M)$ we have

$$\omega\left(\exp\Big(i\hat{\phi}(f)\Big)\right) = \exp\Big(-\frac{1}{2}\mu(f, f)\Big),$$

where both sides of the equation should be interpreted as a power series expansion and the equality should hold for each order of f.

It should be noted that via polarization formulas all n-point functions of a quasi-free state are uniquely defined by the relation above. In particular

$$w_2(f, g) = \mu(f, g) + \frac{i}{2}\sigma_M(f, g).$$

Each quasi-free state can be uniquely associated with a one-particle structure.

Definition 16. *Given the presymplectic space* $(\mathcal{D}(M), \sigma_M)$ *a* one-particle structure (K, H) *is given by a Hilbert space* H *and a real linear map* $K : \mathcal{D}(M) \to H$ *such that* $K(\mathcal{D}(M)) + iK(\mathcal{D}(M))$ *is dense in* H*,* $K \circ (\Box - V) = 0$ *and*

$$2Im(\langle Kf, Kg\rangle) = \sigma_M(f, g).$$

Clearly each one-particle structure defines a quasi-free state via

$$\mu(f, g) = Re(\langle Kf, Kg\rangle),$$

and hence $w_2(f, g) = \langle Kf, Kg\rangle$. That each quasi-free state defines a unique one-particle structure, is proven in [41, Appendix A].

For a general state ω on an algebra $\mathcal{A}$ one can find a unique representation (up to unitary equivalence) $(\mathfrak{H}_\omega, \mathfrak{D}_\omega, \pi_\omega, \Omega_\omega)$ such that $\mathfrak{H}_\omega$ a Hilbert space, $\mathfrak{D}_\omega \subset \mathfrak{H}_\omega$ a dense subset, $\pi_\omega : \mathcal{A} \to L(\mathfrak{D}_\omega)$ a *-homomorphism and $\Omega_\omega \in \mathfrak{D}_\omega$ a unit-vector with $\pi_\omega(\mathcal{A})\Omega_\omega$ dense in $\mathfrak{H}_\omega$ such that

$$\omega(a) = \langle \Omega, \pi_\omega(a)\Omega\rangle.$$

This representation can be obtained using the GNS construction, see for instance [1, Chapter 5]. For quasi-free states on our algebra $\mathcal{A}(M)$ these representations take a special form.

Definition 17. *For* M *globally hyperbolic, a* (bosonic) Fock-space representation $(\mathfrak{H}, \pi)$ *of* $\mathcal{A}(M)$ *is given by a Hilbert space of the form*

$$\mathfrak{H} = \bigoplus_{n=0}^{\infty} S_n\left(H^{\otimes n}\right),$$

where (K, H) *is some one-particle structure on* $(\mathcal{D}(M), \sigma_M)$*,* $H^{\otimes 0} = \mathbb{C}$ *and* $S_n : H^{\otimes n} \to H^{\otimes n}$ *the symmetrization operator, where the inner product* $\langle .,.\rangle_n$ *on* $S_n(H^{\otimes n})$ *is given by*

$$\langle a, b\rangle_0 = \overline{a}b,$$

and for $n > 0$

$$\left\langle \sum_{i_1,\dots,i_n} a_{i_1,\dots,i_n}\psi_{i_1}\dots\psi_{i_n}, \sum_{j_1,\dots,j_n} b_{j_1,\dots,j_n}\phi_{j_1}\dots\phi_{j_n}\right\rangle_n = \sum_{i_1,j_1\dots i_n,j_n} \overline{a_{i_1,\dots,i_n}} b_{j_1,\dots,j_n}\langle\psi_{i_1},\phi_{j_1}\rangle\dots\langle\psi_{i_n},\phi_{j_n}\rangle,$$

*and a *-homomorphism* π *mapping* $\mathcal{A}(M)$ *into the unbounded operators on* $\mathfrak{H}$ *such that*

$$\pi(\hat{\phi}(f)) = \hat{a}(Kf) + \hat{a}(Kf)^*,$$

with

$$\hat{a}(f)^*(\Psi_0, ..., \Psi_n, 0, ...) = (0, S_1(Kf \otimes \Psi_0), ..., S_{n+1}(Kf \otimes \Psi_n), 0, ...).$$

We see that the creation and annihilation operators, $a(\psi)^*$ and $a(\psi)$ respectively (for some $\psi \in H$) satisfy the canonical commutation relations

$$[a(\psi), a(\phi)] = 0, \ [a(\psi)^*, a(\phi)^*] = 0, \ [a(\psi), a(\phi)^*] = \langle \psi, \phi \rangle.$$

If one constructs the Fock space as a representation of the Weyl algebra, one sees immediately that this representation is faithful from the fact that Weyl algebras are simple (see [42, Theorem 5.2.8]) However for completeness we give a direct proof for Fock space representations of $\mathcal{A}(M)$.

Proposition 14. *The Fock space representations of a linear scalar field theory $\mathcal{A}(M)$ for M globally hyperbolic are faithful, i.e. for each $b \in \mathcal{A}(M)$,*

$$\pi(b) = 0 \iff b = 0.$$

Proof. First note that for $f \in \mathcal{D}(M)$ $Kf = 0$ if and only if $\hat{\phi}(f) = 0$. This follows from the fact that $Kf = 0$ implies $\sigma(f, g) = 0$ for all $g \in \mathcal{D}(M)$ which means $f \in (\Box - V)\mathcal{D}(M)$.

Now suppose $b \in \mathcal{A}(M)$. Without loss of generality there are a finite number $f_j \in \mathcal{D}(M)$ for $j = 1, ..., N$ such that $\psi_j = Kf_j \in H$ linearly independent and an $M \in \mathbb{N}$ such that

$$b = \sum_{k_1,...k_N=0}^{M} c_{k_1,...,k_N} (\hat{\phi}(f_1))^{k_1} ... (\hat{\phi}(f_N))^{k_N},$$

which means

$$\pi(b) = \sum_{k_1,...k_N=0}^{N} c_{k_1,...,k_N,l_1,...,l_N} (a(\psi_1)^* + a(\psi_1))^{k_1} ... (a(\psi_N)^* + a(\psi_N))^{k_N}.$$

Note that $H_N = \text{span}(\psi_1, ..., \psi_N)$ is an N-dimensional Hilbert space, on which we can find a basis $\{\phi_j \in H_N : j = 1, ..., N\}$ such that

$$\langle \psi_j, \phi_j \rangle = \delta_{ij}.$$

Assume that $\pi(b) = 0$. This must in particular mean that $[\pi(b), A] = 0$ for any linear operator A on $\mathfrak{H}$. Defining

$$D_A(B) = [A, B],$$

we can now calculate

$$c_{M,...,M} = (D^M_{a(\phi_1)} \circ ... \circ D^M_{a(\phi_N)})(\pi(b)) = 0.$$

This can be repeated for all lower order contributions to yield $c_{k_1,...,k_N} = 0$. Thus $b = 0$. $\square$

A key conceptual result (see for instance [1, Chapter 5]) is that the class of Fock-space representations (up to unitary equivalence) exactly matches the class of GNS representations for a quasi-free state ω per the correspondence of quasi-free states to one-particle structures. Here of course $\mathfrak{H}_\omega = \mathfrak{H}$ and $\pi_\omega = \pi$, but furthermore $\Omega_\omega = (1, 0, ...)$ and $\mathfrak{D}_\omega = \pi(\mathcal{A}(M))\Omega_\omega$. These representations allow for a particle interpretation where $\hat{a}(\psi)$ can be interpreted as creating a particle in the one particle state $\psi \in H$ (taken to be a unit vector) such that we can define number operators $N(\psi) = \hat{a}^*(\psi)\hat{a}(\psi)$, whose eigenvectors can be interpreted as corresponding to states where a finite number of particles in the one-particle state ψ have been excited from the vacuum state Ω_ω. The eigenvalue then corresponds to the number of these particles. In the absence of sufficient symmetries there is generally no clear way to select a preferred particle interpretation and associated vacuum state, after all for free scalar fields of Minkowski space-time a preferred Fock-space representation is selected by the fact that it allows a unitary implementation of space-time symmetries that leave particle numbers invariant. Nevertheless we still see the fact that a theory allows for Fock-spaces and particle interpretations in the first place as a very useful, if not necessary feature of a (linear scalar) quantum field theory. Therefore in section 3, where we discuss the construction of linear scalar quantum fields on semi-globally hyperbolic space-times, we demand that these theories allow for Fock-space representations and in fact use the one-particle structures as a main ingredient for the construction of our theories.

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II. Hadamard states on spherically symmetric characteristic surfaces, the semi-classical Einstein equations and the Hawking effect

Outline

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Summary of Publication

For a linear scalar quantum field theory $\mathcal{A}(M)$ on a globally hyperbolic spacetime M, quasi-free Hadamard states ω defined on some subalgebra $\mathcal{A}(M;U)$ associated with some light-cone interior $U = I^+(p)$ for $p \in M$ can be constructed from particular bi-distributions $\lambda \in \mathcal{D}'(C \times C)$ on cones $C = \partial U \setminus \{p\}$ via a characteristic initial value problem for the equation of motion associated with the theory. This work investigates these bi-distributions, under the requirement that the induced Hadamard state on $\mathcal{A}(M;U)$ may be extended to the full spacetime. For simplicity, only spherically symmetric spacetimes and characteristic cones centred at the axis of symmetry are considered.

The extendibility requirement on the Hadamard state ω fully fixes the singular behaviour of boundary two-point function λ, the general form of which can be deduced from the known local singular behaviour of Hadamard two-point functions on M. However, the precise singular contributions to λ can also be derived from first principles in this setting. In particular, assuming

the metric takes the form

$$\mathrm{d}s^2 = \exp(2\beta(t,r))\left(-\exp(2\alpha(t,r))\mathrm{d}t^2 - 2\mathrm{d}t\mathrm{d}r + r^2\mathrm{d}\Omega^2\right), \tag{II.1}$$

then for a characteristic surface $C_T = \{t = T,\, r > 0\}$, the Hadamard state ω relates to the boundary two-point function λ via

$$\omega(\Phi(f)\Phi(g)) = \lambda(RG_-(f)\restriction_{C_T}, RG_-(g)\restriction_{C_T}), \tag{II.2}$$

for $f, g \in \mathcal{D}(I_+(C_T))$, G_- the retarded propagator associated with the equation of motion and $R = r\exp(\beta)$. For each $N \in \mathbb{N}$ one can explicitly construct a bi-distribution $h_T^{(N)} \in \mathcal{D}'(C_T \times C_T)$ such that

$$\begin{aligned}\lambda(F,G) =& h_T^{(N)}(F,G)\\ &+ \int_{C_T} \mathrm{d}r\mathrm{d}\Omega \int_{C_T} \mathrm{d}r'\mathrm{d}\Omega'\, RR' w_T^{(N)}(r,\Omega;r',\Omega')\partial_r F(r,\Omega)\partial_{r'}G(r',\Omega'),\end{aligned} \tag{II.3}$$

where the function $w_T^{(N)} \in C^{2N+1}(C_T \times C_T)$ is the state-dependent contribution to λ. It is shown how locally, $h_T^{(N)}$ corresponds to the standard Hadamard parametrix modulo some smooth contributions. This allows one to calculate expectation values of renormalized non-linear observables, such as Wick squares and the stress-energy tensor, in the state ω at the surface C_T directly in terms of the function $w_T^{(N)}$ (for sufficiently large N).

Subtracting $h_T^{(N)}$ from λ yields a regularization procedure for two-point functions restricted to light-cones which, in contrast to standard Hadamard subtraction, is globally defined. More specifically, for some Hadamard state ω on $\mathcal{A}(M)$, we can extract a family of two-point functions $t \mapsto w_t^{(N)} \in C^{2N+1}(C_t \times C_t)$. The functions $w_t^{(N)}$ satisfy a dynamical equation which allows one to express $w_t^{(N)}$ in terms of $w_T^{(N)}$ whenever $t \geq T$. In the context of semi-classical Einstein equations, this means that, assuming spherical symmetry, one can reduce the problem of finding a solution to this equation to solving three equations involving the functions α, β and $w_t^{(1)}$, namely the dynamical equation for $w_t^{(1)}$ and two functionally independent components of the Einstein equations. This allows one to formulate a characteristic initial value problem for the semi-classical Einstein equations, which should be further analysed to establish (local) existence of solutions.

As a more concrete application of the developed methods, it is shown how the dynamical equation for $w_t^{(N)}$ can be used to calculate expectation values of non-linear observables on a fixed background given some initial quantum state. This is illustrated by calculating the linear contribution to $\langle :\Phi^2: \rangle$ in terms of a background geometry parameter. Nevertheless, this calculation can be generalized to more involved observables such as the stress-energy tensor. In principle, these methods can also be used to go beyond the linearized contributions, either via analytic or numerical methods. Although one expects these calculations to become quite involved in general, one should be able to derive estimates on these non-linear observables.

Author's contribution

The setting and approach has been discussed and agreed upon by RV and DWJ. Any calculations and derivations have been worked out by DWJ.

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Hadamard states on spherically symmetric characteristic surfaces, the semi-classical Einstein equations and the Hawking effect

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Abstract

We investigate quasi-free Hadamard states defined via characteristic initial data on null cones centred at the axis of symmetry in spherically symmetric space-times. We characterize the necessary singular behaviour of null boundary two-point functions such that one can define non-linear observables at this null boundary and give formulas for the calculation of these observables. These results extend earlier characterizations of null boundary states defining Hadamard states in the bulk of the null cone. As an application of our derived formulas, we consider their implications for the semi-classical Einstein equations and calculate the vacuum polarization associated with Hawking radiation near a collapsing body.

1 Introduction

For many purposes, it can be argued that Hadamard states form the preferred class of physical states on a linear scalar quantum field theory, see for instance Ref. [1]. In particular, it is for this class of states that the expectation value of non-linear observables, such as the (renormalized) stress-energy tensor can be evaluated. A Hadamard state can be characterized by the singular behaviour of its n-point functions. As for a quasi-free Hadamard state it is in particular the two-point function that specifies the state on the entire algebra of linear observables, it is also the singular behaviour of this two-point function, as a bi-distribution on a space-time, that captures the Hadamard property. This singular behaviour can be characterized in multiple ways, most notably via an explicit asymptotic expansion of the integral kernel associated with the two-point function, as given in Ref. [2], or equivalently via the microlocal spectrum condition, as shown in Ref. [3]. That these definitions are equivalent, is most neatly shown if we do not only consider the class of two-point functions of Hadamard states, but the slightly more general notion of a Hadamard paramatrices. In section 3 we will recall the precise characterisation of a Hadamard parametrix in terms of its asymptotic expansion as well as recalling the microlocal spectrum condition and the role of the commutation relation and equation of motion in this definition.

On space-times that admit some characteristic Cauchy surface as a boundary, Hadamard states can be constructed using a bulk to boundary correspondence between the linear observables in the domain of dependence of this boundary surface and an algebra of observables that can be defined on this surface, as used in Ref. [4]. In asymptotically flat space-times these ideas can be extended to conformal boundaries, in particular the past or future null boundary of this space-time, as shown in Ref. [5]. As we will recall in more detail in Sec. 2.3, on these boundary states one can consider an analogue of the microlocal spectrum condition that guarantees the induced state in the bulk to be Hadamard. This allows one to define expectation values for this state of locally covariant non-linear observables in the bulk, such as Wick squares and time-ordered products as defined in Ref. [6] and [7]. However, generally such expectation values diverge near the boundary and hence this state cannot be extended as a Hadamard state across this null boundary. We shall argue that this is related to the fact that, unlike the situation for bulk Hadamard parametrices, the wave front set condition formulated in Ref. [4] does not uniquely fix the singular behaviour of boundary two-point functions. We therefore introduce a necessary condition for extendibility of the bulk Hadamard state in section 3 to explicitly derive the singular part of the boundary two-point function.

For the resulting class of boundary states, we can now show that non-linear observables near the boundary indeed remain finite. In Section 4 we derive explicit formulas for various non-linear observables at the boundary given a boundary two-point function. We shall show how these formulas are particularly useful in the context of semi-classical gravity if one wishes to study the semi-classical Einstein equations as a characteristic initial value problem.

As a further application, in Sec. 5 we shall also give a computation a Wick square expectation value of a quantum field near a gravitationally collapsing body. We shall also comment on how these methods can be generalized to calculate the contribution of the 'Hawking radiation' produced in gravitational collapse to components of the (expectation value of the) stress-energy tensor near the collapsing body. These calculations may open the way to a new understanding of the Hawking effect and black hole evaporation in the context of semi-classical gravity.

2 Basic ingredients from geometry and field theory

For simplicity we will for now restrict our attention to spherically symmetric set-ups. Further generalizations we deem a priori possible, albeit calculationally heavy.

2.1 Geometrical set-up

We consider a space-time M (assumed to be globally hyperbolic) that is spherically symmetric and admits global coordinates $(t, r, \Omega) : M \to \mathbb{R} \times \mathbb{R}_{\geq 0} \times S^2$ (where this map defines a chart almost everywhere, in particular with the exception of the axis of symmetry $r = 0$). We assume that in these coordinates the metric is of the form

$$\mathrm{d}s^2 = -\exp(2(\alpha + \beta))\mathrm{d}t^2 + \exp(2\beta)(-2\mathrm{d}r\mathrm{d}t + r^2\mathrm{d}\Omega^2), \tag{4}$$

where α, β are functions of t, r. Note that in the limiting case that $\alpha = 0$, this space-time is conformally flat, hence we shall refer to this coordinate system as quasi-conformal coordinates. We should also point out that, as can be read off from for instance the formula for the Ricci scalar $\mathfrak{R}$, that not all smooth functions α, β are compatible with a space-time that is smooth at $r = 0$. These regularity conditions shall be addressed when they become relevant for computations.[1]

[1] Admittedly this coordinate system differs from standard choices made to parameterize spherically symmetric space-times. In more conventional choices the coordinate r is either chosen to be an affine parameter for null geodesics (see for instance Ref. [8]) or is chosen such that the volume of a two-sphere at $r = R$ has surface area $4\pi R^2$ (see Ref. [9]). In the latter case, where the metric has the form

$$\mathrm{d}s^2 = -A^2\mathrm{d}t^2 - B^2\mathrm{d}R\mathrm{d}t + R^2\mathrm{d}\Omega^2, \tag{5}$$

a coordinate transformation that brings the metric into the form of eq. (4) (assuming asymptotic flatness for simplicity) is given by

$$r(t, R) = \left(\int_R^\infty \mathrm{d}R \frac{B^2}{R^2}\right)^{-1}. \tag{6}$$

We refer to the point with $t = T, r = 0$ as $p_T \in M$ and the hypersurface $t = T, r \neq 0$ as C_T. The globally hyperbolic space-time $t > T$ will be denoted as $M_T := I^+(C_T)$. Following Ref. [9] we introduce a local null tetrad $(e_i)_{i=0,\dots,3}$, defined away from $r = 0$ by

$$e_0 = \partial_t - \frac{1}{2}\exp(2\alpha)\partial_r, \; e_1 = \exp(-2\beta)\partial_r, \tag{7}$$

and $(e_2, e_3) = (r\exp(\beta))^{-1}(\zeta_1, \zeta_2)$, where (ζ_1, ζ_2) form a local orthonormal frame of $T_\Omega S^2$ (with standard metric $\mathrm{d}\Omega^2$). Using this frame we can write

$$g^{\mu\nu} = \eta^{ab} e_a^\mu e_b^\nu, \tag{8}$$

where η_{ab} is the Minkowski metric expressed in double null coordinates, i.e.

$$\eta^{ab} = \eta_{ab} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

This set-up is sketched in Fig. II.1.

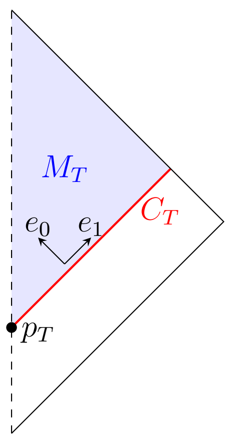

Figure II.1: A Penrose diagram sketching the geometric set-up

We can see that C_T is a characteristic (i.e. null) hypersurface ruled by the bicharacteristics generated by e_1, i.e. the null geodesics $\gamma_{T,\Omega} : (0, \infty) \to C_T$ satisfying

$$\gamma_{T,\Omega}(\lambda) = (T, r(\lambda), \Omega), \; \frac{\mathrm{d}r}{\mathrm{d}\lambda} = \exp(-2\beta(T, r(\lambda))), \; \lim_{\lambda \downarrow 0} r(\lambda) = 0. \tag{10}$$

Note in particular that e_1 is both tangent and orthogonal to C_T. However, as e_1 is a null vector, it can not be normalized. Furthermore, as the induced metric on C_T is degenerate, one cannot use it directly to define a sensible $\mathbb{R}$-valued hypersurface element on C_T to be used as an integration measure. Nevertheless, the vector hypersurface element, that for a spacelike smooth surface Σ is defined as

$$\mathrm{d}\mathbf{S} = \mathrm{d}x\mathrm{d}y\mathrm{d}z\sqrt{h}\mathbf{n}, \tag{11}$$

with $\mathbf{n}$ the future directed normal vector to Σ and h the determinant of the induced metric on Σ (in coordinates (x, y, z)), can be generalized to null hypersurfaces as C_T. Using for instance a limiting procedure where C_T is approached by space-like hypersurfaces, one finds that in our quasi-conformal coordinates, this vector hypersurface element takes the form

$$\mathrm{d}\mathbf{S} = \mathrm{d}r\mathrm{d}\Omega r^2 \exp(2\beta)\partial_r. \tag{12}$$

As we will see in Sec. 2.3, this vector valued integral measure naturally appears in the Klein-Gordon inner product, or alternatively the symplectic structure, for solutions to the Klein Gordon equation on M_T.

2.2 The classical equation of motion for the scalar field

On the space-times introduced above, we consider a real scalar quantum field theory. In particular, we consider a quantization of the real scalar field theory given by the equation of motion

$$(\Box - m^2 - \xi\mathfrak{R})\phi =: P\phi = 0, \tag{13}$$

where classically we typically take $\phi \in \mathcal{E}(M)$ as a smooth function.[2] Here m is some mass parameter, ξ a dimensionless coupling, $\mathfrak{R}$ the Ricci curvature scalar and $\Box$ the Laplace-Beltrami operator given by

$$\Box\phi = \nabla_\mu \nabla^\mu \phi = \frac{1}{\sqrt{|g|}}\partial_\mu(\sqrt{|g|}g^{\mu\nu}\partial_\nu\phi), \tag{14}$$

with ∇ the Levi-Civita connection. In our coordinate system (and using the vectorfields e_0, e_1 as derivations), we can rewrite the sourced equation of motion $P\phi = f \in \mathcal{D}(M)$ as

$$2(e_1 \circ e_0)(r\exp(\beta)\phi) = \left((r\exp(\beta))^{-2}\Delta_\Omega - \tilde{V}\right) r\exp(\beta)\phi - r\exp(\beta)f, \tag{15}$$

[2] After quantization, the quantum field Φ can be seen to live in the space of 'operator valued distributions' (or more generally, distributions taking values in a *-algebra) instead of smooth functions.

where $\tilde{V}$ is a modified potential and $(e_1 \circ e_0)f = e_1^\mu \partial_\mu \left(e_0^\nu \partial_\nu f\right)$.

$$\tilde{V} = m^2 + \xi\mathfrak{R} - 2(r\exp(\beta))^{-1}(e_1 \circ e_0) r \exp(\beta). \tag{16}$$

Note that this additional term to the modified potential is reminiscent of the Ricci scalar, which equals

$$\begin{aligned}\mathfrak{R} =& 12(r\exp(\beta))^{-1}(e_1 \circ e_0) r \exp(\beta) \\ & - 2\exp(2(\alpha - \beta)) \left(\frac{1 - \exp(-2\alpha)}{r^2} - \frac{2\partial_r \alpha}{r} + 2(\partial_r \alpha)^2 + \partial_r^2 \alpha \right). \end{aligned} \tag{17}$$

In fact we can write

$$\begin{aligned}\tilde{V} =& m^2 + \left(\xi - \frac{1}{6}\right) \mathfrak{R} \\ & - \frac{1}{3}\exp(2(\alpha - \beta)) \left(\frac{1 - \exp(-2\alpha)}{r^2} - \frac{2\partial_r \alpha}{r} + 2(\partial_r \alpha)^2 + \partial_r^2 \alpha \right), \end{aligned} \tag{18}$$

from which we can see that for a conformally coupled field, i.e. with $\xi = \frac{1}{6}$, on a conformally flat background, i.e. where $\alpha = 0$, the modified potential takes the simple form $\tilde{V} = m^2$. Due to frequent appearance in the rest of this paper, it is convenient to define

$$R(t, r) := r \exp(\beta(t, r)). \tag{19}$$

Defining the differential operator on $\mathcal{E}(C_T)$

$$K_T = \frac{1}{2}\left[\exp(2\beta(T, r))\tilde{V}(T, r) - \frac{1}{r^2}\Delta_\Omega - \partial_r \exp(2\alpha(T, r))\partial_r\right], \tag{20}$$

we can shortly write the sourced equation of motion as

$$(\partial_r \partial_t + K_t) R\phi = -\frac{R}{2} f. \tag{21}$$

It is this form of the (sourced) Klein-Gordon equation that we shall use in most of the following considerations.[3]

2.3 Quantum field theoretic set-up

As alluded to in the introduction, we can consider a quantum field theory to live equivalently on the bulk M_T or on the boundary C_T. We shall quickly introduce both these viewpoints.

[3]We shall often drop the subscript t from K_t when it is clear from context at what surface C_t it is meant to operate.

The bulk theory

We use the framework of algebraic quantum field theory, in particular using the model for the free real scalar quantum field due to Ref. [10] in the formulation used for instance in Ref. [11]. In order to fix conventions and notation, we shall quickly sketch the definition of the algebra of linear observables $\mathcal{A}(M)$ on the space-time M. This is a unital *-algebra consisting of polynomials (with complex valued coefficients) over objects of the form $\Phi(f)$ with $f \in \mathcal{D}(M)$ a (real-valued) test function on M such that[4]

- *(linearity)* for $a \in \mathbb{R}$ and $f, g \in \mathcal{D}(M)$ we have
$$\Phi(af + g) = a\Phi(f) + \Phi(g), \tag{24}$$
- *(hermiticity)* for $f \in \mathcal{D}(M)$ we have
$$\Phi(f)^* = \Phi(f), \tag{25}$$
- *(dynamics)* for $f \in \mathcal{D}(M)$ and $P : \mathcal{E}(M) \to \mathcal{E}(M)$ the differential operator defined in eq. (13) we have
$$\Phi(Pf) = 0, \tag{26}$$
- *(CCR)* for $f, g \in \mathcal{D}(M)$ we have
$$[\Phi(f), \Phi(g)] = \mathrm{i}E(f, g). \tag{27}$$

Here $E : \mathcal{D}(M)^2 \to \mathbb{R}$ is the commutator function defined by
$$E(f, g) = \int_M \mathrm{dvol}\, g G_c(f), \tag{28}$$
with $G_c = G_- - G_+$ the causal propagator and $G_\pm$ the unique advanced and retarded propagators given by $PG_\pm(f) = f$ and $\mathrm{supp}(G_\pm(f)) \subset J^\pm(\mathrm{supp}(f))$ (see Ref. [12]).

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[4] One can work equally well with complex test functions, where for $h = f_1 + \mathrm{i}f_2 \in \mathcal{D}(M, \mathbb{C})$ we define
$$\Phi(h) := \Phi(f_1) + \mathrm{i}\Phi(f_2). \tag{22}$$
This means in particular that
$$\Phi(h)^* := \Phi(\overline{h}). \tag{23}$$
The choice for real test functions is here made in accordance with Ref. [2].

A state $\omega : \mathcal{A}(M) \to \mathbb{C}$, which for hermitian operators can be interpreted as mapping the operator onto its expectation value, is a normalized (i.e. $\omega(1) = 1$) positive semi-definite (i.e. $\omega(aa^*) \in \mathbb{R}_{\geq 0}$) complex-linear map. In this work we restrict ourselves to quasi-free (or Gaussian) states, defined uniquely by their two-point functions

$$\Lambda(f, g) := \omega(\Phi(f)\Phi(g)), \tag{29}$$

typically taken to be (complex valued) bi-distributions on $\mathcal{D}(M)$, where all higher order n-point functions are calculated via Isserlis theorem (see Ref. [13]). As reviewed in the same reference, such a two point function must have the properties

- $\Lambda \circ (P \otimes 1) = \Lambda \circ (1 \otimes P) = 0$,
- $Re \circ \Lambda$ is a positive semi-definite symmetric real bilinear map on $\mathcal{D}(M)^2$,
- $Im \circ \Lambda = \frac{1}{2}E$,
- $|E(f, g)|^2 \leq 4\Lambda(f, f)\Lambda(g, g)$.

In fact any bi-distribution satisfying the properties above defines a quasi-free state.

Quasi-free states are said to satisfy the (local) Hadamard condition if on any Cauchy normal neighbourhood $U \subset M$ the two-point function has an asymptotic expansion of a 'fundamental solution' to $P_x\Lambda(x, y) = 0$

$$\Lambda \sim \frac{1}{8\pi^2}\left[\frac{u}{\sigma_+} + \sum_{n=0}^{\infty} v^{(n)}\sigma^n \ln\left(a^{-2}\sigma_+\right) + w^{(n)}\sigma^n\right]. \tag{30}$$

Here σ is the Synge world function, a an arbitrary length scale and $u, v^{(n)}, w^{(n)}$ are smooth functions satisfying certain transport equations, which can be derived from $P\Lambda(x, y) = 0$ (see Ref. [14] or Sec. 3). The (local) bi-distribution $\frac{1}{\sigma_+}$ (and similarly $\ln(\sigma_+)$) is defined on $\mathcal{D}(U)$ as

$$\left(\frac{1}{\sigma_+}\right)(f, g) = \lim_{\varepsilon \downarrow 0} \int_U \mathrm{dvol}_x \int_U \mathrm{dvol}_y \frac{f(x)g(y)}{\sigma(x, y) + \mathrm{i}a\varepsilon(\mathcal{T}(x) - \mathcal{T}(y)) + a^2\varepsilon^2}, \tag{31}$$

where $\mathcal{T}$ is an arbitrary time-function on M. In the following sections we shall often write this as

$$\sigma_+(f, g) = \sigma(f, g) + \mathrm{i}0^+(\mathcal{T}(x) - \mathcal{T}(y)) + \left(0^+\right)^2. \tag{32}$$

A more complete discussion on this definition, including many subtleties that are not addressed here, can be found in Ref. [2]. Here it should be noted that some technical details in the extension of the local definition above to global Hadamard states, defined on a region larger than a Cauchy normal neighbourhood, have been addressed only recently in Ref. [15].

As first shown in Ref. [3], the Hadamard condition can also be formulated in the language of microlocal analysis (see Appendix A). A two-point function is Hadamard if and only if it satisfies the microlocal spectrum condition, i.e. for its wave front set we have

$$WF'(\Lambda) = \Big\{((x_1,k_1),(x_2,k_2)) \in (T^*(M)\setminus \mathbf{0})^2 : (x_1,k_1)\sim(x_2,k_2), k_1 \in \left(V^+_{x_1}\right)^d\Big\}, \quad (33)$$

where $\left(V^+_{x_1}\right)^d$ is the dual of the closed future light cone. This alternative characterization has proven very useful for studying general properties of Hadamard states, and can be nicely generalized beyond the scalar field in 3+1 dimensions, as seen for instance in Ref. [16]. While we will not make direct use of tools from microlocal analysis, in later sections we definitely rely on results on Hadamard states derived from this reformulation. Still, we deem a detailed discussion of the wave front set mentioned above beyond the scope of this text. In essence, the wave front set captures aspects of the singular ultraviolet behaviour of a (bi-)distribution, generalizing the singular support of a distribution. It is important to keep in mind that any arbitrary bi-distribution satisfying the microlocal spectrum condition will generally not have the asymptotic expansion give in eq. (30). As theorem 5.1 in Ref. [3] indicates, to really establish the two-way connection between this expansion and the microlocal spectrum condition, one needs the equation of motion $\Lambda\circ(P\otimes 1) = \Lambda\circ(1\otimes P) = 0$ and the commutation relation $Im(\Lambda) = \frac{1}{2}E$, or rather, that these identities hold up to smooth integral kernel. Hence a bi-distribution satisfying the microlocal spectrum condition, and

$$WF'(\Lambda\circ(P\otimes 1)) = WF'(\Lambda\circ(1\otimes P)) = WF'\left(Im(\Lambda) - \frac{1}{2}E\right) = \emptyset, \quad (34)$$

can be referred to as a Hadamard parametrix. Notably, the fact that a two-point function is positive semi-definite is not required in the theorem cited above. In fact, theorem 6.3 of the same reference tells us that positivity (again modulo a smooth function) is automatically satisfied for a Hadamard parametrix.

The most well-known example of a Hadamard state is the Minkowski vacuum state for free theories on flat space-time, but in fact any ground- or thermal (i.e. KMS) state on a static space-time satisfies the microlocal specrum condition (see Ref. [17] and [18]). A state satisfying the Hadamard condition in a neighbourhood of a Cauchy surface will satisfy the Hadamard condition on the whole space-time, hence the existence of Hadamard states on any globally hyperbolic space-time can be asserted from existence on static space-times using a deformation argument (see Ref. [19]). One can also give existence results via a direct construction as performed in Ref. [20].

The boundary theory

For each $T \in \mathbb{R}$ we can consider the algebra $\mathcal{A}_T := \mathcal{A}(M; M_T)$.[5] Clearly, these algebras satisfy $\mathcal{A}_T \subset \mathcal{A}_{T'}$ for any $T' \leq T$. Following Ref. [4] we can also associate an algebra $\mathcal{B}_T$ with the characteristic surface C_T such that $\mathcal{A}_T \cong \mathcal{B}_T$, which we view as a bulk to boundary correspondence, in the way described below.

Recalling the definition of R in eq. (19) and that of the causal propagator G_c in section 2.3, we define the map $\rho_T : \mathcal{D}(M_T) \to \tilde{\mathcal{S}}_{s.c.}(C_T) \subset \mathcal{E}(C_T)$ via

$$\rho_T(f) = RG_c(f)\restriction_{C_T}, \tag{35}$$

where $\tilde{\mathcal{S}}_{s.c.}(C_T)$ is defined such that this map is surjective. As proven in Ref. [21],

$$\rho_T(f) = \rho_T(g) \text{ implies } G_c(f)\restriction_{M_T} = G_c(g)\restriction_{M_T}, \tag{36}$$

and hence, by theorem 3.4.7 in Ref. [12], $f - g \in P\mathcal{D}(M_T)$. This means that $\rho_T : \mathcal{D}(M_T)/P\mathcal{D}(M_T) \to \tilde{\mathcal{S}}_{s.c.}(C_T)$ is a linear isomorphism.

We can define a symplectic structure σ_{C_T} on $\tilde{\mathcal{S}}_{s.c.}(C_T)$ via

$$\sigma_{C_T}(F, G) = 2\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega\, F\partial_r G. \tag{37}$$

This is chosen such that the map ρ_T becomes a symplectomorphism, as using the form of the Klein-Gordon equation in eq. (21), we can see that for $f, g \in \mathcal{D}(M_T)$

$$\begin{aligned} E(f,g) = &\int_{M_T} \mathrm{dvol}\, gG_c(f) \\ =&2\int_T^\infty \mathrm{d}t \int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega\, RG_c(f)\left[-\partial_t\partial_r - K_t\right] RG_-(g) \\ =&2\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega\, \left[RG_c(f)\partial_r RG_-(g)\right]\restriction_{C_T} + \int_{M_T} \mathrm{dvol}\, G_-(g)PG_c(f) \\ =&2\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega\, \rho_T(f)\partial_r\rho_T(g) \\ =&\sigma_{C_T}(\rho_T(f), \rho_T(g)), \end{aligned} \tag{38}$$

[5] For any open set $U \subset M$, the localized algebra $\mathcal{A}(M; U) \subset \mathcal{A}(M)$ is defined as the smallest unital *-algebra such that for any $f \in \mathcal{D}(U)$ (understood as a subset of $\mathcal{D}(M)$) we have $\Phi(f) \in \mathcal{A}(M; U)$.

where we have used that K_T is symmetric on $\tilde{\mathcal{S}}_{s.c.}(C_T)$ when given the $L^2(C_T, \mathrm{d}r\mathrm{d}\Omega)$ inner product, that near $r = 0$ we have $RG_c(g) = \mathcal{O}(r)$ and that $RG_c(g)$ is spatially compact, i.e. there is an $\tilde{r} > 0$ such that $\mathrm{supp}(RG_c(g)\restriction_{C_T}) \subset \{r < \tilde{r}\}$.

Completely analogously to as in section 2.3, we can now construct an algebra $\mathcal{B}_T$ generated by elements $\Psi(F)$ for $F \in \tilde{\mathcal{S}}_{s.c.}(C_T)$ satisfying

- $\Psi(aF + G) = a\Psi(F) + \Psi(G)$,
- $\Psi(F)^* = \Psi(F)$,
- $[\Psi(F), \Psi(G)] = \mathrm{i}\sigma_{C_T}(F, G)$.

The symplectomorphism ρ_T induces a natural *-isomorphism $\iota_T : \mathcal{A}_T \to \mathcal{B}_T$ via

$$\iota_T(\Phi(f)) = \Psi(\rho_T(f)). \tag{39}$$

Note that while the dynamics of the theory is implemented in (the net structure of) $\mathcal{A}_T$, we cannot say the same for $\mathcal{B}_T$. The latter theory can only be seen as dynamical by virtue of its bulk to boundary correspondence. However, as we will see in section 3.1, we can also understand this dynamics in terms of the family of algebras $\{\mathcal{B}_T : T \in \mathbb{R}\}$ and their relations.

Clearly, just as on $\mathcal{A}_T$, we can define quasi-free states on $\mathcal{B}_T$ using the 2-point function $\lambda_T : \tilde{\mathcal{S}}_{s.c.}(C_T)^2 \to \mathbb{C}$ satisfying

- $Re \circ \lambda_T$ is a positive definite symmetric real bilinear map,
- $Im \circ \lambda_T = \frac{1}{2}\sigma_{C_T}$,
- $|\sigma_{C_T}(F, G)|^2 \leq 4\lambda_T(F, F)\lambda_T(G, G)$.

A two-point function λ_T can be used to define a two-point function Λ_T on $\mathcal{D}(M_T)$ via

$$\Lambda_T(f, g) = \lambda_T(\rho_T(f), \rho_T(g)). \tag{40}$$

Reversely, given a two-point function Λ on $\mathcal{D}(M)$, we can give a formal expression for λ_T such that $\Lambda_T = \Lambda\restriction_{\mathcal{D}(M_T)^2}$ via

$$\lambda_T(r, \Omega; r', \Omega') = 4\partial_r\partial_{r'}R(T, r)R(T, r')\Lambda(T, r, \Omega; T, r', \Omega'). \tag{41}$$

Here $\Lambda(x; x')$ is the (formal) integration kernel of Λ (with respect to the volume measure induced by the metric) and $\lambda_T(r, \Omega; r', \Omega')$ the formal integration kernel of λ_T (with respect to the (hypersurface) area element $\mathrm{d}r\mathrm{d}\Omega$). This relation can be derived from noting that for $f, g \in \mathcal{D}(M_T)$

$$\Lambda(f,g) = \int_{M_T} \mathrm{dvol}_x f(x)\Lambda(x,g) = \sigma_{C_T}(R\Lambda(.,g)\restriction_{C_T}, \rho_T(f)). \tag{42}$$

Of course this only holds if $\Lambda(., g)$ is sufficiently regular. As also noted in Ref. [2], the formal relation (41) cannot be made precise for arbitrary distributions. Luckily, we can make sense of this expression for Hadamard states. That is to say, as we will see in section 3, to do this one needs an appropriate choice of time-function in the definition of $\frac{1}{\sigma_+}$.

As was shown in Ref. [4], a two-point function λ_T induces a Hadamard two-point function Λ_T on $\mathcal{D}(M_T)$ if it satisfies the *characteristic micro-local spectrum condition* (cμSC):

- ${}_{C_t}WF'(\lambda_t) = WF'(\lambda_t)_{C_t} = \emptyset$,
- $WF'(\lambda_t) \cap \{((r,\Omega),(\sigma,\xi);(r',\Omega'),(\sigma',\xi')) \in T^*(C_t \times C_t) : \sigma > 0 \text{ or } \sigma' > 0\} = \emptyset$,

where we identify $T^*_{(r,\Omega)}C_t \cong \mathbb{R} \times T^*_\Omega S^2$. Here we again point to appendix A for the relevant definitions and notation regarding the wave front set. Notably, these conditions do not fully fix the singular behaviour of λ_T, i.e. for two boundary two-point functions, λ_T and λ'_T, satisfying the cμSC, their difference $\lambda_T - \lambda'_T$ need not be smooth. This is contrast with what we know for Hadamard two-point functions on the bulk. If we consider Λ_T and Λ'_T, their difference $\Lambda_T - \Lambda'_T$ has a smooth integral kernel on M_T^2. However, this kernel may generally not be extendible as a smooth function to M^2 (and hence may not define a smooth function on C_T^2 via equation (41)). Here lies the reason that the cμSC on λ_T doesn't fix the singular behaviour, as this condition does not guarantee that Λ_T can be extended as a Hadamard two-point function to all of M, or at the very least to a neighbourhood of C_T. Physically, this has as a consequence that for these states the expectation values of observables such as the stress-energy tensor may blow up as one approaches C_T from above. Contrastingly, suppose that λ_T and λ'_T define two-point functions Λ_T and Λ'_T that *can* be extended as Hadamard bi-distributions to all of $\mathcal{D}(M)$, we have in particular that

$$(\Lambda_T - \Lambda'_T)\restriction_{C_T^2}(r,\Omega;r',\Omega') := \lim_{t\downarrow T}(\Lambda_T - \Lambda'_T)(t,r,\Omega;t,r',\Omega') \tag{43}$$

exists and is a smooth function. This in turn implies that

$$(\lambda_T - \lambda'_T)(r,\Omega;r',\Omega') = 4\partial_r\partial_{r'}RR'(\Lambda_T - \Lambda'_T)\restriction_{C_T^2}(r,\Omega;r',\Omega') \tag{44}$$

is smooth. Hence λ_T and λ'_T have the same singular behaviour. It is this class of boundary two-point functions that we shall refer to as *characteristic Hadamard two-point functions.*

The characteristic Hadamard two-point functions shall be the main object of study in section 3. Arguably the most immediate question is what the singular behaviour, given for instance in terms of an asymptotic expansion analogous to eq. (30), is for these states.[6] This question is relevant if one wants to consider the semi-classical Einstein equations in terms of a characteristic initial value problem. Here one considers some initial state on a characteristic surface such that at least the stress-energy tensor is well-defined at this surface. One method to determine this singular behaviour would be via an explicit calculation of λ_T from some global Hadamard two-point function Λ using (41). This is done for the vacuum state of a massless field on Minkowski space-time in Ref. [2]. However for general spherically symmetric space-times this can be rather tedious, as it for instance requires us to know the behaviour of σ, the Synge world function, and of u in a neighbourhood of the null geodesics that rule C_T. In this paper we take an alternative approach that, arguably, allows us to determine the necessary singular behaviour of λ_T from first principles. We will see in section 3 that the main benefit of this approach is that it automatically yields us a *characteristic Hadamard parametrix* h_T, i.e. a bi-distribution defined globally on C_T such that for each characteristic Hadamard function λ_T the difference $\lambda_T - h_T$ is smooth. As we will discuss in section 4.1, this yields a point splitting procedure to renormalize operators such as the stress-energy tensor with some particularly nice behaviour (compared to directly point splitting with regards to a Hadamard parametrix that is locally constructed). In particular, this procedure generalizes the point-splitting procedure on conformally flat space-times discussed in Ref. [22].

3 The characteristic Hadamard parametrix

The asymptotic expansion of Hadamard states in eq. (30) allows one to locally define (order N) Hadamard parametrices

$$H_N = \frac{1}{8\pi^2}\left[\frac{u}{\sigma_+} + \sum_{n=0}^{N} v^{(n)}\sigma^n \ln\Big(a^{-2}\sigma_+\Big)\right], \tag{45}$$

[6]In principle one could consider feeding eq. (30) directly into eq. (41). However, this would typically not give a globally defined parametrix, nor would the restriction of σ to C_T^2, at least on a neigbourhood where it is defined, be a convenient object to work with.

such that $\Lambda - H_N$ has an $2N+1$ times continuously differentiable distribution kernel, which modulo a C^{2N+1} contribution is uniquely determined by requiring that $H_N \circ (P \otimes 1)$ is $2N-1$ times continuously differentiable and $u(x,x) = 1$.[7] In particular, following Ref. [14], or for a more recent and timely account, Ref. [23], one can use the defining relations of the Synge world function

$$\nabla_\mu \sigma \nabla^\mu \sigma = 2\sigma,\ \sigma(x,x) = 0, \tag{46}$$

where the covariant derivatives are understood to act on the first coordinate, to derive that H_N is a parametrix if u and $v^{(n)}$ satisfy the following *transport equations*

$$2\nabla^\mu \sigma \nabla_\mu \ln(u) + \Box\sigma - 4 = 0, \tag{47}$$

$$v^{(0)} + \nabla^\mu \sigma \left(\nabla_\mu v^{(0)} - v^{(0)} \nabla_\mu \ln(u)\right) + \frac{1}{2} P u = 0, \tag{48}$$

$$(n+2) v^{(n+1)} + \nabla^\mu \sigma \left(\nabla_\mu v^{(n+1)} - v^{(n+1)} \nabla_\mu \ln(u)\right) + \frac{1}{2(n+1)} P v^{(n)} = 0. \tag{49}$$

Given $u(x,x) = 1$ this system of equations is uniquely solved on Cauchy normal neighbourhoods, in particular we get $u = \sqrt{\Delta}$ with Δ the van Vleck-Morette determinant. Furthermore, it has been shown in Ref. [24] that the functions u and $v^{(n)}$, the latter of which are referred to as the Seeley-DeWitt (or sometimes Hadamard) coefficients, are symmetric.[8] A further important feature of these coefficients, and hence of H_N, is that they are locally covariant. That is, for fixed mass m and curvature coupling ξ, $u(x,x')$ and $v^{(n)}(x,x')$ only depend on the geometry of a geodesically convex neighbourhood of x and x'. This is why the order N Hadamard parametrices can be used to give locally covariant definitions of non-linear observables for this quantum field theory, such as the stress-energy tensor, via a point-splitting procedure (see

[7] Strictly speaking, these are not Hadamard parametrices in the sense of how we described them in section 2.3, as the P acting on H_N generally does not yield a smooth function, however for many purposes, especially when defining non-linear observables of finite order, such an 'approximate' notion of a Hadamard parametrix is sufficient.

[8] In actual fact, there is some ambiguity in the choice of transport equations, or more generally in the definition of the Seeley-deWitt coefficients. For instance, the function u can in principle be modified freely by any $\mathcal{O}(\sigma)$ contribution. However, for any Hadamard parametrix H_N with the desired properties, these ambiguities only lead to $2N+1$-times continuously differentiable differences in the definition and are hence often irrelevant. The coefficients defined by the transport equations above are seen as the canonical choice, though of course even in this case, the bi-distributions H_N still contain a further ambiguity in the choice of reference scale a.

Ref. [6]).

We wish to do an analogous computation to construct a characteristic Hadamard parametrix in terms of functions that one can naturally define on a characteristic hypersurface.[9] Recall that in order for the μSC to imply the Hadamard condition for a bi-distribution, we need to impose a dynamical requirement, i.e. that it satisfies the equation of motion up to a smooth source, and that it is consistent with the (singular part of the) commutation relation. Comparing this to the cμSC, the commutation relation can be imposed at the boundary, and the dynamical requirement inside the bulk is imposed via the bulk to boundary correspondence. However, we do not have a dynamical requirement at the boundary itself, the bulk two-point function need not satisfy the equation of motion at a point on the characteristic boundary (or, as two-point functions are distributional, rather on 'test functions' that are non-zero at some boundary submanifold). Hence, in order to derive the singular structure of characteristic Hadamard two-point functions, we shall impose a condition on these boundary two-point functions that is related to the equation of motion being satisfied at this boundary. We implement this dynamical requirement on boundary two-point functions via the evolution of these two-point functions over the family of characteristic surfaces $\{C_t : t \in \mathbb{R}\}$, as outlined in the following section.

3.1 The dynamics of boundary two-point functions

Suppose that Λ is a Hadamard two-point function on M. Let λ_t be the family of boundary two-point functions on C_t such that

$$\Lambda\restriction_{\mathcal{D}(M_t)^2} = \Lambda_t = \lambda_t \circ (\rho_t \otimes \rho_t). \tag{50}$$

For $f, g \in \mathcal{D}(M_t)$ we can always find a $t' > t$ such that $f, g \in \mathcal{D}(M_{t'})$. This means that $\Lambda_t(f, g) = \Lambda_{t'}(f, g)$. In particular

$$\partial_t \Lambda_t(f, g) = 0. \tag{51}$$

Using the bulk to boundary correspondence, we find that this implies

$$0 = \partial_t \Lambda_t(f, g) = \dot{\lambda}_t(\rho_t(f), \rho_t(g)) + \lambda_t(\dot{\rho}_t(f), \rho_t(g))) + \lambda_t(\rho_t(f), \dot{\rho}_t(g))) = 0. \tag{52}$$

[9] For two points on a characteristic surface that are not placed on the same bicharacteristic, i.e. the null curves generated by the vectorfield e_1, the functions σ, u and v_n depend highly non-trivially on the surrounding geometry of the surface. We aim to find an expansion describing the same singular behaviour that is more adapted to our characteristic approach.

Due to the fact that $G_c(f)$ has compact spatial support, we can integrate the classical equation of motion (21) to write

$$\dot{\rho}_t(f)(r,\Omega) = \int_r^\infty \mathrm{d}s\,(K_t\rho_t(f))(s,\Omega). \tag{53}$$

Formally, we can use this to write down a dynamical equation for the integration kernel $\lambda_t(r,\Omega;r',\Omega')$, namely

$$\dot{\lambda}_t(r,\Omega;r',\Omega') + K_t\int_0^r \mathrm{d}s\,\lambda_t(s,\Omega;r',\Omega') + K_t'\int_0^{r'} \mathrm{d}s\,\lambda_t(r,\Omega;s,\Omega') = 0, \tag{54}$$

where K_t should be interpreted as acting on the unprimed coordinates (and be dependent on r) and K_t' on the primed coordinates, and depending on r'.[10]

On our class of spherically symmetric space-times with quasi-conformal coordinates as given in Sec. 4, we now wish to find a family of bi-distributions h_t on $\mathcal{S}_{s.c.}(C_t)$ that satisfy the cμSC, the commutation relation and such that

$$\dot{h}_t + h_t\circ(O_t\otimes 1) + h_t\circ(1\otimes O_t) = -4S_t, \tag{55}$$

for some family of functions $S_t\in\mathcal{E}(M^2)\restriction_{C_t^2}$ smooth in t and where the map $O_t:\mathcal{S}_{s.c.}(C_t)\to C^\infty(C_t)$ is given by

$$O_t(f)(r,\Omega) = \int_r^\infty \mathrm{d}s\,(K_tf)(s,\Omega). \tag{56}$$

Given some fixed T, we now consider a bulk two-point function $\Lambda_T = \lambda_T\circ(\rho_T\otimes\rho_T)$ such that its corresponding boundary two-point function satisfies

$$\lambda_T = h_T + 4\partial_r\partial_r' RR'w_T, \tag{57}$$

with

$$w_T\in\mathcal{E}(M^2)\restriction_{C_T^2}. \tag{58}$$

This bulk two-point function Λ_T defines a family of boundary two point functions $\{\lambda_t\}_{t\geq T}$, via the state induced on $\mathcal{B}_t\cong\mathcal{A}_t\subset\mathcal{A}_T$. We now claim that

$$\lambda_t - h_t\in\partial_r\partial_{r'}RR'\mathcal{E}(M^2)\restriction_{C_t^2}, \tag{59}$$

and hence we can find a $w_t\in\mathcal{E}(M^2)\restriction_{C_t^2}$ with

$$w_t(r,\Omega;r',\Omega') = \frac{1}{4RR'}\int_0^r \mathrm{d}s\int_0^{r'}\mathrm{d}s'\,(\lambda_t - h_t)(s,\Omega;s',\Omega). \tag{60}$$

[10]See appendix B for a derivation of this equation.

In particular, such a w_t should satisfy

$$(\partial_t\partial_r\partial_{r'} + K_t\partial_{r'} + K'_t\partial_r)\, RR'w_t = S_t. \tag{61}$$

Indeed, given a w_t satisfying equation (61) for $t > T$, with w_T determined from Λ_T, then we can see that the family $\lambda_t = h_t + 4\partial_r\partial_{r'}RR'w_t$ satisfies $\partial_t\Lambda_t(f, g) = 0$ for any $f, g \in \mathcal{D}(M_t)$. Now we can easily conclude that

$$\Lambda_t(f, g) = \Lambda_T(f, g). \tag{62}$$

The question that remains, is whether eq. (61) indeed has smooth solutions. To show this, we write

$$w_t(r, \Omega; r', \Omega') = w_{t,T} + \int_T^t \mathrm{d}s\, F_{t,s}(r, \Omega; r', \Omega'), \tag{63}$$

where for $t > T$

$$(\partial_t\partial_r\partial_{r'} + K_t\partial_{r'} + K'_t\partial_r)\, RR'w_{t,T} = 0, \tag{64}$$

and for $t > s \geq T$

$$(\partial_t\partial_r\partial_{r'} + K_t\partial_{r'} + K'_t\partial_r)\, RR'F_{t,s} = 0, \tag{65}$$

such that

$$\lim_{t\downarrow T} w_{t,T} = w_T, \tag{66}$$

and

$$\lim_{t\downarrow s} F_{t,s} = \frac{1}{RR'}\int_0^r \mathrm{d}r \int_0^{r'} \mathrm{d}r' S_s. \tag{67}$$

For this latter boundary condition, it is important to note that $\frac{1}{RR'}\int_0^r \mathrm{d}r \int_0^{r'} \mathrm{d}r' S_s$, as well as all of its derivatives in r and r', can be continuously extended to $r = 0$ and $r' = 0$.

For $t > s \geq T$, both $w_{t,T}$ and $F_{t,s}$ exist and are smooth, as they can be given as restrictions to C_t^2 of the (smooth) integral kernel of

$$4\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega'\, \rho_T(f)(r, \Omega)\rho_T(g)(r', \Omega')\partial_r\partial_{r'}RR'w_T(r, \Omega; r', \Omega'), \tag{68}$$

and

$$4\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega'\, \rho_s(f)(r, \Omega)\rho_s(g)(r', \Omega')S_s(r, \Omega; r', \Omega'), \tag{69}$$

respectively.[11] To show that w_t exists and is smooth, we first note that $F_{t,s}$ is continuous as a function of s. After all, we have that $\partial_s F_{t,s}$ is the restriction to C_t^2 of the integration kernel of

$$-\int_0^\infty \mathrm{d}r \int_{S^2} \mathrm{d}\Omega \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega' \, \rho_s(f)(r,\Omega)\rho_s(g)(r',\Omega') \times \left[\dot{S}_s(r,\Omega;r',\Omega') + K \int_0^r \mathrm{d}r \, S_s(r,\Omega;r',\Omega') + K' \int_0^{r'} \mathrm{d}r' \, S_s(r,\Omega;r,\Omega') \right]. \tag{70}$$

Therefore, as $\partial_s F_{t,s}$ exists as a smooth function of $(r,\Omega;r',\Omega')$ for all $s<t$, we know that $F_{t,s}$, as well as all its derivatives in r, r', Ω and Ω', are continuous as a function of s. Furthermore, as both $F_{t,t}$ and $F_{t,T}$ exist as smooth functions on C_t^2, then for all fixed $(r,\Omega;r',\Omega')$, we know that $F_{t,s}$ is bounded on $s \in [T,t]$ and hence (Riemann) integrable. Hence we know that w_t exists and that furthermore, by the Leibniz integral rule, we know that w_t is smooth.

To construct a characteristic Hadamard parametrix satisfying the dynamical condition (55) in the same vain as how one could construct H_N, we wish to make an Ansatz about the form of h_t. To understand which Ansatz to make, it is helpful to consider a simple class of space-times and quantum field theories on which the full singular structure of characteristic Hadamard states is known explicitly.

A relevant example: the conformal vacuum

On a conformally flat spherically symmetric space-time (i.e. $\alpha = 0$), we consider a massless conformally coupled scalar field ($m=0$, $\xi = \frac{1}{6}$). For such a theory we can define the conformal vacuum state (see for instance Ref. [22]) via

$$\Lambda(t,r,\Omega;t',r',\Omega') = \frac{1}{4\pi^2}\left[\frac{\exp(-\beta(t,r)-\beta(t',r'))}{-(t-t')^2 - 2(t-t'-\mathrm{i}0^+)(r-r'-\mathrm{i}0^+) + 2rr'(1-\cos(\theta))}\right], \tag{71}$$

[11] That these integral kernels are smooth, can be seen from simple analogues to the proof of theorem 5.3 in Ref. [4], where in this case we have for the initial data that $WF'(\partial_r\partial_{r'}RR'w_T) = WF'(S_s) = \emptyset$.

where θ is the relative angle between Ω and Ω'.[12] Notably on Minkowski space-time this just matches the Minkowski vacuum state

$$\Lambda(t, r, \Omega; t', r', \Omega') = \frac{1}{8\pi^2 \sigma_+}. \tag{73}$$

Doing a calculation completely analogous to the derivation of eq. (B.53) in Ref. [2], we see that the conformal vacuum boundary two-point functions are given by

$$\lambda_t(r, \Omega; r', \Omega') = \frac{-1}{\pi} \frac{\delta_{S^2}(\Omega, \Omega')}{(r - r' - \mathrm{i}0^+)^2}. \tag{74}$$

Fur such a boundary two-point function, one can indeed show that eq. (54) holds.

3.2 An Ansatz for the singular behaviour of characteristic Hadamard states

If we consider an arbitrary scalar field on a non-conformally flat space-time, the two-point functions of eq. (74) still satisfies the cμSC and is has an imaginary part that yields the correct commutation relations. Hence, it defines a Hadamard two-point functions Λ_t on M_t. In fact, for states of this form this was already proven in Ref. [8]. If we calculate $\partial_t \Lambda_t$ for this family of states (see Appendix B), we find that

$$\partial_t \Lambda_t(f, g) = \frac{1}{\pi} \int \mathrm{d}r \mathrm{d}r' \mathrm{d}\Omega \, \rho_t(f)(r, \Omega) \rho_t(g)(r', \Omega) \kappa_t^{(0)}(r, r'), \tag{75}$$

[12]Note that the time-function that is chosen here to regularize the integral kernel of this state is given by $\mathcal{T} = r + t$, which is indeed time-like as

$$g(\nabla \mathcal{T}, \nabla \mathcal{T}) = -\exp(-2\beta). \tag{72}$$

This temporal function is chosen such that in the calculation of λ_t, one need not worry about time-splitting, i.e. doing the calculation on $C_t \times C_{t+0^+}$, in order for (41) to yield a well-defined distribution. When one simply chooses $\mathcal{T} = t$, the calculation of λ_t would yield an expression for the integration kernel where integrals diverge in the limit $\varepsilon \downarrow 0$. This technicality is discussed in Ref. [2].

with

$$
\begin{aligned}
2\kappa_t^{(0)}(r,r') :=& \frac{\exp(2\beta_t(r'))\tilde{V}(r') - \exp(2\beta_t(r))\tilde{V}(r)}{r'-r} \\
&+ \frac{r\exp(2\beta_t(r))\tilde{V}(r) + r'\exp(2\beta_t(r'))\tilde{V}(r')}{rr'} \\
&- 2\frac{\exp(2\alpha(r')) - \exp(2\alpha(r))}{(r'-r)^3} \\
&+ \frac{\partial_r \exp(2\alpha(r)) + \partial_{r'}\exp(2\alpha(r'))}{(r'-r)^2}.
\end{aligned} \tag{76}
$$

In particular, we see that the boundary integral kernel of $\partial_t\Lambda_t$ is singular, as it contains a δ_{S^2}-like behaviour.[13] Aside from this singular behaviour in the angular coordinates, we can see that for smooth space-times, $\kappa_t^{(0)}$ is in fact smooth at $r = r' > 0$ (or rather has a unique smooth extension to this submanifold). That being said, in general this $\kappa^{(0)}$ still diverges near $r = 0$ or $r' = 0$. We wish to use eq. (74) as the leading order singularity in our Ansatz, so we will need to find additional lower order singular terms to ensure that $\partial_t\Lambda_t$ has a smooth boundary integral kernel. Analogous to the bulk Hadamard expansion, we make the following Ansatz,

$$
\lambda_t(r,\Omega;r',\Omega') = \frac{-1}{\pi}\frac{\delta(\Omega,\Omega')}{(r-r'-\mathrm{i}0^+)^2} + \frac{1}{2\pi^2}\partial_r\partial_{r'}R(t,r)R(t,r')\tilde{\lambda}_t(r,\Omega;r',\Omega'), \tag{77}
$$

with

$$
\tilde{\lambda}_t = w_t + v_t \ln\left(\frac{RR'(1-\cos\theta)}{a^2}\right). \tag{78}
$$

Here we assume that $w_t, v_t \in \mathcal{E}(M^2)\restriction_{C_T^2}$. Note that the logarithmic divergences precisely coincide with pairs of points on C_t that are located on a bicharacteristic. This is why it is reasonable to expect that these logarithmic divergences match those of Λ when restricted to C_t^2, i.e. that v_t is related to the Hadamard coefficients $\{v^{(n)} : n \in \mathbb{N}\}$. We will verify this explicitly in section 4. If we consider purely our dynamical conditions on characteristic Hadamard states, the appearance of these logarithmic divergences is also

[13]At first glance it may seem surprising that there are no terms containing $\Delta_\Omega\delta_{S^2}$ appearing in this distribution. After all, the operator K contains a term involving the operator Δ_Ω. However, as we see in Appendix B, this term indeed vanishes upon close inspection. The fact that this term does not contribute for a relatively simple two-point function, is a feature of our chosen of coordinates. For more general forms of the metric, one sees that the leading order singular term of the characteristic Hadamard expansion has to be modified into a more complicated form to get the same result.

natural, as here we see that

$$\Delta_\Omega \ln(1-\cos\theta) = 4\pi\delta_{S^2}(\Omega,\Omega') - 1. \tag{79}$$

It is this relation that allows us to cancel all singularities appearing in $\partial_t\Lambda_t$ when v_t is chosen such that it satisfies certain transport equations.

3.3 The transport equations for the characteristic Hadamard coefficients

Similarly to the bulk Hadamard states, v_t should be state-independent and geometrical. That means in particular that it should respect the symmetries of the space-time, which enables us to formally expand v_t as

$$v_t(r,\Omega;r',\Omega') = \sum_{n=0}^{\infty} v_t^{(n)}(r,r')(1-\cos\theta)^n. \tag{80}$$

In principle, we don't know a priori if this expansion is absolutely convergent, but at least one can interpret this as an asymptotic expansion. Notably, unlike the asymptotic expansion in eq. (30), this expansion is unique.[14] We shall refer to $v_t^{(n)}$ as the *characteristic Hadamard coefficients.*

[14]Recall our comment on the ambiguity of $v^{(n)}$ in footnote 8.

This expansion allows us to rewrite the condition $\partial_t \Lambda_t = 0$ as

$$
\begin{aligned}
0 =& \partial_r \partial_{r'} \partial_t R R' \tilde{\lambda}_t - \frac{1}{2} \Delta_\Omega \left[\frac{R}{r^2} \partial_{r'} R' \tilde{\lambda}_t + \frac{R'}{r'^2} \partial_r R \tilde{\lambda}_t \right] \\
&+ \frac{1}{2} \Big[\Big(\exp(2\beta) \tilde{V} - \partial_r \exp(2\alpha) \partial_r \Big) R \partial_{r'} R' \tilde{\lambda}_t \\
&+ \Big(\exp(2\beta') \tilde{V}' - \partial_{r'} \exp(2\alpha') \partial_{r'} \Big) R' \partial_r R \tilde{\lambda}_t \Big] \\
&+ 2\pi \kappa_t^{(0)} \delta_{S^2} \\
=& 2\pi \left(\kappa^{(0)} - 2 \frac{R'}{r'^2} \partial_r R v_t^{(0)} \right) \delta_{S^2} + \\
& \sum_{n=0}^{\infty} (n+1)^2 (1 - \cos\theta)^n \ln\Big(a^{-2} R R' (1 - \cos\theta) \Big) \Big[\kappa_t^{(n+1)} - 2 \frac{R'}{r'^2} \partial_r R v_t^{(n+1)} \Big] \\
&+ (1 - \cos\theta)^n \Big[\frac{1}{RR'} \partial_t R R' \partial_r \partial_{r'} R R' v_t^{(n)} \\
&+ \partial_t ((\partial_r R)(\partial_{r'} R') v_t^{(n)} - R R' \partial_r \partial_{r'} v_t^{(n)}) \\
&+ \frac{R'}{r'^2} \partial_r R \left((2n+1) v_t^{(n)} - 4(n+1) v_t^{(n+1)} \right) \\
&+ \frac{R'}{r'^2} (\partial_r R) \left(n(n+1) v_t^{(n)} - 2(n+1)^2 v_t^{(n+1)} \right) \\
&+ \Big(\exp(2\beta) \tilde{V} - \partial_r \exp(2\alpha) \partial_r \Big) R (\partial_{r'} R') v_t^{(n)} \\
&- \partial_r \exp(2\alpha) (\partial_r R) \partial_{r'} R' v_t^{(n)} - \frac{(\partial_r R)}{R} \exp(2\alpha) \partial_r R \partial_{r'} R' v_t^{(n)} \Big] \\
&+ (\partial_t \partial_r \partial_{r'} + K_t \partial_{r'} + K'_t \partial_r) R R' \tilde{w}_t + (r \leftrightarrow r'),
\end{aligned} \tag{81}
$$

with

$$
\begin{aligned}
\kappa_t^{(n+1)} =& \frac{1}{2(n+1)^2} \Big[\partial_t \partial_r \partial_{r'} R R' v_t^{(n)} + \Big(\exp(2\beta) \tilde{V} - \partial_r \exp(2\alpha) \partial_r \Big) R \partial_{r'} R' v_t^{(n)} \\
&+ (n+1) n \frac{R'}{r'^2} \partial_r R v_t^{(n)} \Big] + (r \leftrightarrow r').
\end{aligned} \tag{82}
$$

We can read off the transport equation

$$
\left[\frac{R}{r^2} \partial_{r'} R' + \frac{R'}{r'^2} \partial_r R \right] v_t^{(n)} = \kappa_t^{(n)}, \tag{83}
$$

which has the unique solution (demanding $v_t^{(n)}$ to be finite at $r = 0$ and $r' = 0$)

$$
v_t^{(n)}(r, r') = \frac{(rr')^2}{RR'} \int_0^\infty \mathrm{d}s \, \frac{\kappa^{(n)} \left(\frac{r}{1+rs}, \frac{r'}{1+r's} \right)}{(1+rs)^2 (1+r's)^2}. \tag{84}
$$

We arrive at the conclusion that for characteristic Hadamard states, the asymptotic expansion of v_t is uniquely determined by the geometry near the lightcone C_t. The remaining smooth part w_t is state-dependent and satisfies the dynamical equation

$$(\partial_t \partial_r \partial_{r'} + K_t \partial_{r'} + K'_t \partial_r) R R' w_t = S_t \tag{85}$$

with

$$\begin{aligned} S_t = -\frac{1}{2} \sum_{n=0}^{\infty} (1 - \cos\theta)^n \Bigg[& \frac{1}{RR'} \partial_t R R' \partial_r \partial_{r'} R R' v_t^{(n)} \\ & + \partial_t \left((\partial_r R)(\partial_{r'} R') v_t^{(n)} - R R' \partial_r \partial_{r'} v_t^{(n)} \right) \\ & + \frac{R'}{r'^2} \partial_r R \left((2n+1) v_t^{(n)} - 4(n+1) v_t^{(n+1)} \right) \\ & + \frac{R'}{r'^2} (\partial_r R) \left(n(n+1) v_t^{(n)} - 2(n+1)^2 v_t^{(n+1)} \right) \\ & + (\partial_{r'} R') \left(\exp(2\beta) \tilde{V} - \partial_r \exp(2\alpha) \partial_r \right) R v_t^{(n)} \\ & - \frac{1}{R} (\partial_r R) \exp(2\alpha) \partial_r \partial_{r'} R R' v_t^{(n)}) \\ & - \partial_r \exp(2\alpha) (\partial_r R) \partial_{r'} R' v_t^{(n)}) \\ & + (r \leftrightarrow r') \Bigg]. \end{aligned} \tag{86}$$

Note that S_t is independent of the reference scale a introduced in the logarithmic part of the two-point function. Hence one sees that for each Hadamard distribution where the smooth part w_t satisfies Eq. (85), one directly finds a whole family of Hadamard bi-solutions parameterized by a. However, it should be noted that these distributions in general do not define a two-point function, as for arbitrary reference scale a this map may not be positive semi-definite.

For general space-times and couplings the source term above is somewhat unwieldy. It is likely not possible to write it in a closed form, or even find a comprehensive formula for each term in the expansion. Luckily, calculating the expansion of the source-term above to some finite order is still useful when wanting to calculate certain coincidence limits of w_t, as discussed in Sec. 5. Nevertheless, in some simple cases we can find formulas for the terms in the expansion to arbitrary order, for which we shall give a non-trivial example of below.

3.4 Example: the massive field on Minkowski space-time

On Minkowski space-time, i.e. $\alpha = \beta = 0$, we consider a scalar field with mass m. In particular, this means that $\tilde{V} = m^2$. For quasi-free states satisfying the Ansatz (77) we find that

$$\kappa_t^{(0)} = \frac{m^2}{2}\left(\frac{1}{r} + \frac{1}{r'}\right). \tag{87}$$

This implies that $v_t^{(0)} = \frac{m^2}{2} = v^{(0)}$, where $v^{(0)}$ is the Seeley-DeWitt coefficient given by the transport equations from the beginning of this section. This is a good first indication that our findings are consistent with the known expansion of the Hadamard singularity. More generally, using also that our space-time is time-translation invariant, we see that our recurrence relation given by (82) and (83) simplify to

$$\begin{aligned}\kappa_t^{(n+1)} = \frac{1}{2(n+1)^2}\Bigg[&\left((m^2 - \partial_r^2)\partial_{r'} + (m^2 - \partial_{r'}^2)\partial_r\right) rr' v_t^{(n)} \\ &+ n(n+1)\left(\frac{1}{r^2}\partial_{r'} + \frac{1}{r'^2}\partial_r\right) rr' v_t^{(n)}\Bigg],\end{aligned} \tag{88}$$

$$\left[\frac{1}{r^2}\partial_{r'} + \frac{1}{r'^2}\partial_r\right] rr' v_t^{(n)} = \kappa_t^{(n)}. \tag{89}$$

Making the further Ansatz

$$v_t^{(n)} = \frac{m^2}{2} a_n (m^2 rr')^n, \tag{90}$$

we calculate

$$\kappa^{(n+1)} = \frac{m^2}{2}\frac{a_n}{2(n+1)}(m^2 rr')^{n+1}\left(\frac{1}{r} + \frac{1}{r'}\right), \tag{91}$$

and see that the recurrence relation reduces to

$$a_n = \frac{a_{n-1}}{2(n+1)n}, \tag{92}$$

hence

$$a_n = \frac{1}{2^n n!(n+1)!}. \tag{93}$$

In fact, we can use the dynamical equation (85) to (almost fully) specify the smooth part of the vacuum state. We note that for the source term S_t we have

$$S_t = \left(\frac{1}{r} + \frac{1}{r'}\right)\frac{m^2}{2}\sum_{n=0}^{\infty}(m^2 rr')^{n+1}(1-\cos\theta)^n \frac{2n+3}{2^{n+1}n!(n+2)!}. \tag{94}$$

The vacuum state ought to be invariant under continuous Poincaré transformations. This means in particular that in the bulk two-point function the only dependence on space-time points enters via the Synge world function σ and (time)-orientation, where the latter is of particular relevance in the commutator. The Hadamard coefficients $v_t^{(n)}$ found above define a (bulk) Hadamard parametrix that indeed respects these symmetries. This means that the smooth part of the two-point function ought to do the same. Therefore the function w_t is a function of $\sigma\restriction_{C_t^2} = rr'(1-\cos\theta)$, hence we make the Ansatz

$$w_t = \frac{m^2}{2}\sum_{n=0}^{\infty} b_n (m^2 rr'(1-\cos\theta))^n, \tag{95}$$

we find that (85) yields

$$\left(\frac{1}{r} + \frac{1}{r'}\right)\frac{m^2}{2}\sum_{n=0}^{\infty}(m^2 rr')^{n+1}(1-\cos\theta)^n \frac{n+1}{2}(b_n - 2(n+1)(n+2)b_{n+1}) = S_t, \tag{96}$$

from which one can deduce the relation

$$b_{n+1} = \frac{b_n}{2(n+1)(n+2)} - a_{n+1}\frac{2n+3}{(n+1)(n+2)}. \tag{97}$$

Note that this system of equations needs an initial condition on b_0 to be uniquely solvable. We can then express all coefficients b_n in terms of b_0,

$$b_n = \frac{1}{2^n n!(n+1)!}\left[b_0 - \sum_{j=1}^{n}\frac{2j+1}{j(j+1)}\right] = \frac{1}{2^n n!(n+1)!}\left(b_0 - 2H[n] + \frac{n}{n+1}\right), \tag{98}$$

where $H[n] = \sum_{j=1}^{n}\frac{1}{j}$ are the harmonic numbers. Using the convention $H[0]=0$, we can now write down the full 2-point function of the massive vacuum state

$$\Lambda_m = \frac{1}{8\pi^2}\left[\frac{1}{\sigma_+} + \frac{m^2}{2}\sum_{n=0}^{\infty}\frac{(m^2\sigma)^n}{2^n n!(n+1)!}\left(\ln\left(\frac{\sigma_+}{a^2}\right) - 2H[n] + \frac{n}{n+1}\right)\right], \tag{99}$$

where we have absorbed the unknown b_0 in to the reference scale a. Recalling the remark made below Eq. (86), the reference scale a still needs to be fixed to a particular value such that the bi-distribution above defines a positive semi-definite two-point function. One can show that the expression above can be written in terms of modified Bessel functions. Let $F_c = K_1 + cI_1 \in \mathcal{E}(\mathbb{R}_{>0})$, with I_1 and K_1 modified Bessel functions of the first and second kind respectively and $c \in \mathbb{R}$ an a priori free parameter, such that F_c solves the modified Bessel equation

$$x^2\partial_x^2 F_c(x) + x\partial_x F_c(x) - (x^2+1)F_c(x) = 0. \tag{100}$$

We can now rewrite the expression for Λ_m above as

$$\Lambda_m = \frac{m}{4\pi^2\sqrt{2\sigma^+}} F_c(m\sqrt{2\sigma_+}), \tag{101}$$

where using the known expansions for the modified Bessel functions for $x \downarrow 0$ (see Ref. [25, p. 375])

$$I_1(x) = \frac{1}{2}x + \mathcal{O}(x^2), \tag{102}$$

and

$$K_1(x) = \frac{1}{x} + I_1(x)\ln(x) + \frac{2\gamma - \ln(4) - 1}{4}x + \mathcal{O}(x^2), \tag{103}$$

where γ is the Euler-Masceroni constant, we can relate

$$c = \frac{1}{2}\ln\left(\frac{e^{2\gamma-1}m^2}{2a^2}\right). \tag{104}$$

Of course the two-point function of the proper Minkowski vacuum state is well known, and exactly matches the case where $c = 0$, or $a^2 = \frac{e^{2\gamma-1}m^2}{2}$. To show that this is indeed the unique choice for c such that Λ_m is positive semi-definite, we rely on an argument involving the behaviour of the two-point function at large space-like separation. Write

$$\Lambda_m = \Lambda_{m,0} + cW, \tag{105}$$

where

$$\Lambda_{m,0} = \frac{m}{4\pi^2\sqrt{2\sigma^+}} K_1(m\sqrt{2\sigma_+}) \tag{106}$$

the proper vacuum state two-point function and $W \in \mathcal{E}(M \times M)$ given by

$$W = \frac{m}{4\pi^2\sqrt{2\sigma}} I_1(m\sqrt{2\sigma}). \tag{107}$$

Due to the exponential decay of $K_1(x)$ as $x \to \infty$, we know that $\Lambda_{m,0}$ satisfies the cluster decomposition property (see Ref. [26]). Let $f, g \in \mathcal{D}(\mathbb{R}^4)$ and $\tau_{\mathbf{v}} : \mathcal{D}(M) \to \mathcal{D}(M)$ a translation map for a space-like vector $\mathbf{v}$ given by

$$\tau_{\mathbf{v}} f(\mathbf{x}) = f(\mathbf{x} - \mathbf{v}), \tag{108}$$

where we have identified points on Minkowski space with fourvectors. The cluster decomposition property for this Poincare invariant two-point functions tells us that

$$\lim_{s\to\infty} \Lambda_{m,0}(f + \tau_{s\mathbf{v}} g, f + \tau_{s\mathbf{v}} g) = \Lambda_{m,0}(f, f) + \Lambda_{m,0}(g, g). \tag{109}$$

$I_1(x)$ on the other hand is known to exponentially diverge (to positive infinity) for $x \to \infty$. If we therefore choose $f \in \mathcal{D}(M)$ such that $f \geq 0$ and $f \notin P\mathcal{D}(M)$, one easily sees that for each $B > 0$ there is an $d > 0$ such that for $s > d$

$$W(f, \tau_{s\mathbf{v}} f) > B. \tag{110}$$

Therefore for $c \neq 0$,

$$\Lambda_m(f - c\tau_{s\mathbf{v}} f, f - c\tau_{s\mathbf{v}} f) \to -\infty \text{ as } s \to \infty. \tag{111}$$

we conclude that $c = 0$ is the only possible choice to yield a positive definite two-point function. Hence, using our methods, we regain the expanded form of the vacuum two-point function for the massive scalar field on Minkowski space-time

$$\Lambda_m = \frac{1}{8\pi^2}\left[\frac{1}{\sigma_+} + \frac{m^2}{2}\sum_{n=0}^{\infty}\frac{(m^2\sigma)^n}{2^n n!(n+1)!}\left(\ln\left(\frac{\mathrm{e}^{2\gamma-1}m^2\sigma_+}{2}\right) - 2H[n] + \frac{n}{n+1}\right)\right]. \tag{112}$$

The state studied above is arguably very elementary and well understood, therefore this construction does not really reveal anything new about the massive vacuum state. Nevertheless, it acts as a good consistency check for the methods we have introduced. In the next section, we will show that the characteristic Hadamard parametrix

$$h_t = \frac{-1}{\pi}\frac{\delta_{S^2}(\Omega, \Omega')}{(r - r' - \mathrm{i}0^+)^2} + \frac{1}{2\pi^2}\partial_r\partial_{r'} RR' v_t \ln\Big(a^{-2}RR'(1 - \cos\theta)\Big), \tag{113}$$

although not a locally covariant object, can be a very useful tool when calculating the expectation values of non-linear observables, especially the stress-energy tensor.

4 Wick squares, the stress-energy tensor and all that

We shall now discuss how to use the characteristic parametrix defined in Section 3 to calculate expectation values of renormalized locally covariant non-linear observables such as Wick squares and the stress-energy tensor for a two-point function λ_t on the boundary C_t. Naively, one might define non-linear observables by point-splitting λ_t and subtracting the characteristic parametrix. However, such a procedure generally does not yield a locally covariant renormalization scheme. Instead we require that our observables are defined via a locally covariant renormalization scheme as described in [6]. In particular, the observables are constructed via a point-splitting procedure where a locally covariant Hadamard parametrix H is subtracted. Here we also take note of the finite renormalization ambiguity due to the non-uniqueness of this prescription.[15] We start by calculating a simple Wick square $\langle : \Phi^2 : \rangle$, which for a bulk two-point function Λ is defined as

$$\langle : \Phi^2 : \rangle_\Lambda(x) = \lim_{x' \to x} (\Lambda - H)(x', x) + c_1 m^2 + c_2 \mathfrak{R}(x), \tag{114}$$

where $c_1, c_2 \in \mathbb{R}$ denote the renormalization ambiguities (depending analytically on ξ). If we formally restrict a Hadamard two-point function Λ to C_t^2, we now know that

$$\begin{aligned}\Lambda(t, r, \Omega; t, r', \Omega') = \frac{1}{8\pi^2} \Bigg[&\frac{\exp(-\beta(t, r) - \beta(t, r'))}{\mathrm{i}0^+(r - r' - \mathrm{i}0^+) + rr'(1 - \cos(\theta))} \\ &+ v_t(r, \Omega; r', \Omega') \ln \left(a^{-2} R R' (1 - \cos\theta) \right) \\ &+ w_t(r, \Omega; r', \Omega') \Bigg],\end{aligned} \tag{115}$$

where we recognise the leading order term as the conformal vacuum 2-point function restricted to the cone. We can now use this to rewrite the Wick square as

$$\begin{aligned}8\pi^2 \langle : \Phi^2 : \rangle_\Lambda(t, r, \Omega) =& w_t(r, \Omega; r, \Omega) \\ &+ \lim_{\Omega' \to \Omega} \frac{1}{R^2(1 - \cos(\theta))} - \frac{u(t, r, \Omega; t, r, \Omega')}{\sigma(t, r, \Omega; t, r, \Omega')} \\ &+ \lim_{\Omega' \to \Omega} v_t^{(0)}(r, r) \ln \left(a^{-2} R^2 (1 - \cos\theta) \right) \\ &\quad - v^{(0)}(t, r, \Omega; t, r, \Omega') \ln \left(a^{-2} \sigma(t, r, \Omega; t, r, \Omega') \right) \\ &+ 8\pi^2 \left(c_1 m^2 + c_2 \mathfrak{R}(t, r, \Omega) \right).\end{aligned} \tag{116}$$

[15] In the case of the stress-energy tensor some of this ambiguity is fixed by additional requirements, such as divergencelessness. See Ref. [27].

To show that this is indeed finite, let us first observe that

$$\begin{aligned}\sigma(t,r,\Omega;t,r,\Omega') =&[\partial_\theta^2\sigma](1-\cos\theta)+\frac{1}{6}\left([\partial_\theta^4\sigma]+[\partial_\theta^2\sigma]\right)(1-\cos\theta)^2\\&+\mathcal{O}((1-\cos\theta)^3)\\=&R^2(1-\cos\theta) \quad (117)\\&+\frac{1}{6}R^2(1-(\partial_rR)(\exp(2\alpha)(1+\partial_r\beta)-2r\partial_t\beta))(1-\cos\theta)^2\\&+\mathcal{O}((1-\cos\theta)^3), \quad (118)\end{aligned}$$

and

$$\begin{aligned}u(t,r,\Omega;t,r,\Omega')=&[u]+[\partial_\theta^2u](1-\cos\theta)+\mathcal{O}((1-\cos\theta)^2)\\=&1+\frac{1}{12}(d\Omega)^{\mu\nu}R_{\mu\nu}(1-\cos\theta)+\mathcal{O}((1-\cos\theta)^2), \quad (119)\end{aligned}$$

where we have used the square bracket notation [...] to denote the coincidence limit of a biscalars (see Ref. [28]). It follows that

$$\lim_{\Omega'\to\Omega}\frac{1}{R^2(1-\cos(\theta))}-\frac{u(t,r,\Omega;t,r,\Omega')}{\sigma(t,r,\Omega;t,r,\Omega')}=\frac{[\partial_\theta^4\sigma]+[\partial_\theta^2\sigma]}{6R^4}-\frac{[\partial_\theta^2u]}{R^2}, \quad (120)$$

which is indeed finite.

Turning our attention to the logarithmic divergences, we want to show that $[v_t^{(0)}]=[v^{(0)}]$, which we've already seen to hold for the massive field on Minkowski space-time. Indeed, if we expand the transport equation (83) in powers of $(r'-r)$, equating lowest order terms gives

$$\partial_rR^2[v_t^{(0)}]=r^2[\kappa_t^{(0)}]=\frac{1}{2}\left(\partial_rR^2\tilde{V}+\frac{r^2}{6}\partial_r^3\exp(2\alpha)\right). \quad (121)$$

Using relation (18) for $\tilde{V}$, this differential equation reduces to

$$\partial_rR^2[v_t^{(0)}]=\frac{1}{2}\partial_rR^2\left(m^2+\left(\xi-\frac{1}{6}\right)\mathfrak{R}\right)=\partial_rR^2[v^{(0)}], \quad (122)$$

which indeed asserts that $[v_t^{(0)}]=[v^{(0)}]$.

Putting this all together, we can finalize our computation of $\langle :\Phi^2:\rangle$, which gives

$$\langle :\Phi^2:\rangle_\Lambda\restriction_{C_t}=\frac{1}{8\pi^2}[w_t]+Q_{\Phi^2}, \quad (123)$$

with

$$\begin{aligned}Q_{\Phi^2}=&\frac{(1-6[\partial_\theta^2u])[\partial_\theta^2\sigma]+[\partial_\theta^4\sigma]}{48\pi^2[\partial_\theta^2\sigma]^2}+\text{renormalization freedom}\\=&c_1m^2+\left(c_2-\frac{1}{288\pi^2}\right)\mathfrak{R}-\frac{1}{48\pi^2}\mathbf{C}[e_0,e_1,e_0,e_1]. \quad (124)\end{aligned}$$

Here $\mathbf{C}$ is the Weyl tensor. It should be noted that while Q_{Φ^2} contains the locally covariant renormalization ambiguity, it is not as a whole locally covariant. In particular, the contribution

$$\mathbf{C}[e_0, e_1, e_0, e_1] = -\frac{1}{3R^2}\left(1 - \exp(2\alpha) + r\partial_r \exp(2\alpha) - \frac{1}{2}r^2\partial_r^2 \exp(2\alpha)\right) \tag{125}$$

is a quantity associated with the local null tetrad depending on the chosen lightcone. Of course $[w_t]$ is also not a locally covariant quantity, as it is defined by subtracting the characteristic parametrix from λ_t. As we have defined $\langle : \Phi^2 : \rangle$ such that it as a whole is locally covariant, we will refer to Q_{Φ^2} as the covariance correction term.

As we will encounter the following terms in the stress-energy tensor, we will also calculate the covariance correction terms for

$$\langle : \partial_r\Phi\partial_r\Phi : \rangle = \frac{1}{8\pi^2}[\partial_r\partial_{r'}w_t] + Q_{(\partial_r\Phi)^2}, \tag{126}$$

and

$$\langle : \|\vec{\nabla}_\Omega\Phi\|^2_{S^2} : \rangle = \frac{1}{8\pi^2}[\nabla_\Omega \cdot \nabla_{\Omega'}w_t] + Q_{\|\vec{\nabla}_\Omega\Phi\|^2_{S^2}}, \tag{127}$$

which are calculated analogously to Q_{Φ^2}.[16] We get

$$\begin{aligned}
Q_{(\partial_r\Phi)^2} = &-\frac{R_{rr}\left(m^2 + \left(\xi - \frac{1}{6}\right)\mathfrak{R}\right)}{96\pi^2} - \frac{1}{2880\pi^2}\left(2\nabla_r\nabla_r\mathfrak{R} + R_r{}^\mu R_{\mu r} - \frac{8}{3}R_{rr}\mathfrak{R}\right) \\
&+\frac{1}{2880\pi^2}\Big(- 6\nabla^\alpha\nabla^\beta C_{\alpha r\beta r} - 6\nabla_r\nabla_r\mathbf{C}[e_0, e_1, e_0, e_1] \\
&\qquad + (7R_{rr} - 9(\nabla_\alpha e_1^\alpha)^2(e_0)_r(e_0)_r)\mathbf{C}[e_0, e_1, e_0, e_1]\Big) \\
&+ \text{renormalisation freedom}
\end{aligned} \tag{128}$$

[16]To ease these calculations, we used the xAct packages for Mathematica (see Ref. [29]). The notebooks involving these calculations can be made available upon request.

and

$$
\begin{aligned}
&Q_{\|\nabla_\Omega \Phi\|^2_{S^2}} = \left(d\Omega^2\right)^{\mu\nu} \times \\
&\Bigg[\left(-\frac{R_{\mu\nu}\left(m^2+\left(\xi-\frac{1}{6}\right)\mathfrak{R}\right)}{96\pi^2} - \frac{1}{2880\pi^2}\left(2\nabla_\mu\nabla_\nu\mathfrak{R} + R_\mu{}^\alpha R_{\alpha\nu} - \frac{8}{3}R_{\mu\nu}\mathfrak{R}\right)\right) \\
&+ g_{\mu\nu}\left(\frac{\mathfrak{R}\left(m^2+\left(\xi-\frac{1}{6}\right)\right)}{576\pi^2} - \frac{1}{17280\pi^2}\left(6R^{\alpha\beta\gamma\delta}R_{\alpha\beta\gamma\delta} - \mathfrak{R}^2 - 6R^{\alpha\beta}R_{\alpha\beta}\right)\right) \\
&+ \frac{1}{2880\pi^2}\left(-6\nabla^\alpha\nabla^\beta C_{\alpha\mu\beta\nu} - 6\nabla_\mu\nabla_\nu \mathbf{C}[e_0,e_1,e_0,e_1] + 7R_{\mu\nu}\mathbf{C}[e_0,e_1,e_0,e_1]\right) \\
&+ \frac{1}{960\pi^2}g_{\mu\nu}\Bigg(\Box + 20m^2 + \left(10\xi - \frac{3}{2}\right)\mathfrak{R} - 18\mathbf{C}[e_0,e_1,e_0,e_1] \\
&\qquad\qquad + 5\mathbf{R}[e_0,e_1,e_0,e_1] - 6R^{-2}\Bigg)\mathbf{C}[e_0,e_1,e_0,e_1]\Bigg] \\
&+ \text{renormalisation freedom}
\end{aligned} \tag{129}
$$

4.1 The stress-energy tensor

Classically, the stress energy tensor $\mathbf{T}$ of a linear scalar field (as defined for instance in Ref. [30]) is (in terms of its components) given by

$$
\begin{aligned}
T_{\mu\nu} =& \nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla^\rho\phi\nabla_\rho\phi - \frac{1}{2}g_{\mu\nu}m^2\phi^2 \\
&+ \xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box\right]\phi^2.
\end{aligned} \tag{130}
$$

This object is of main interest in the context of the (classical) Einstein equations

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} = 8\pi T_{\mu\nu}. \tag{131}$$

Similarly, a quantum stress-energy tensor $:\mathbf{T}:$, which for general quantum field theories is related to their relative Cauchy evolution as given in Ref. [31], can be used to write down the semi-classical Einstein equations

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} = 8\pi\langle : T_{\mu\nu} : \rangle, \tag{132}$$

which dynamically couples a quantum field to a background geometry. The solution of such an equation is then given by a (globally hyperbolic) spacetime M and a state ω on $\mathcal{A}(M)$ such that $\langle : T_{\mu\nu} : \rangle$ is evaluated in ω. The classical stress-energy tensor is divergenceless, and for the semi-classical Einstein equations to be consistent, this also needs to hold for the quantum stress-energy tensor,

$$\nabla^{\mu}\langle : T_{\mu\nu} : \rangle = 0. \tag{133}$$

Following the analysis in Ref. [9], we can see that on our class of spherically symmetric space-times there are only two functionally independent components of the stress-energy tensor, that is assuming that $\langle : \mathbf{T} : \rangle$ is smoothly defined on the entire space-time (which is the case if it is evaluated for a Hadamard state). Using our null tetrad introduced in Section 2.1, these independent components are $\langle : \mathbf{T} : \rangle[e_0, e_1]$ and $\langle : \mathbf{T} : \rangle[e_1, e_1]$. Classically these correspond to

$$\begin{aligned}\mathbf{T}[e_0, e_1] =& \frac{1}{2r^2}\exp(-2\beta)\left(\frac{1}{2}\vec{\nabla}^2_{\Omega}\phi^2 - \phi\vec{\nabla}^2_{\Omega}\phi\right) + \frac{1}{2}m^2\phi^2 \\ &+ e_0^{\mu}e_1^{\nu}\xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_{\mu}\nabla_{\nu} + g_{\mu\nu}\Box\right]\phi^2,\end{aligned} \tag{134}$$

and

$$\begin{aligned}\mathbf{T}[e_1, e_1] =& \exp(-4\beta)\left(\frac{1}{2}\partial_r^2\phi^2 - \phi\partial_r^2\phi\right) \\ &+ e_1^{\mu}e_1^{\nu}\xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_{\mu}\nabla_{\nu} + g_{\mu\nu}\Box\right]\phi^2.\end{aligned} \tag{135}$$

In principle $: \mathbf{T} :$ is given in terms of Wick squares $: \Phi^2 :$ and $: \Phi\nabla_{\mu}\nabla_{\nu}\Phi :$, and hence can be renormalized using a point-splitting procedure. However, not every renormalization scheme results in a stress-energy tensor that is divergenceless. Luckily, one can always transform a (locally covariant) renormalization scheme for the stress-energy tensor into a divergenceless definition by making use of the renormalization freedom of locally covariant Wick squares. Following Ref. [27], or a more recent review in Ref. [23], if we denote the stress-energy tensor regularized by point-splitting and subtracting the Hadamard parametrix H by $\mathbf{T}^{\mathrm{reg}}$, the divergenceless quantum stress-energy tensor is given by

$$\langle : T_{\mu\nu} : \rangle = \langle T^{\mathrm{reg}}_{\mu\nu}\rangle + g_{\mu\nu}D + d_1 K^{(1)}_{\mu\nu} + d_2 K^{(2)}_{\mu\nu} + d_3 m^2\left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R}\right) + d_4 m^4 g_{\mu\nu}, \tag{136}$$

with D the divergence correction

$$\begin{aligned}D = \frac{1}{5760\pi^2}\Big(&2R^{\alpha\beta\gamma\delta}R_{\alpha\beta\gamma\delta} - 2R^{\alpha\beta}R_{\alpha\beta} + 5(1-6\xi)^2\mathfrak{R}^2 \\ &+ 12(1-5\xi)\Box\mathfrak{R} - 60m^2(1-6\xi)\mathfrak{R} + 180m^4\Big),\end{aligned} \tag{137}$$

$\mathbf{K}^{(i)}$ the conserved locally covariant geometric tensors of mass dimension 4

$$K^{(1)}_{\mu\nu} = -2\Box R_{\mu\nu} + \frac{2}{3}\nabla_\mu\nabla_\nu\mathfrak{R} + \frac{1}{3}g_{\mu\nu}\Box\mathfrak{R} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + g_{\mu\nu}R_{\alpha\beta}R^{\alpha\beta} + \frac{4}{3}\mathfrak{R}R_{\mu\nu} - \frac{1}{3}g_{\mu\nu}\mathfrak{R}^2, \tag{138}$$

$$K^{(2)}_{\mu\nu} = 2\nabla_\mu\nabla_\nu\mathfrak{R} - 2g_{\mu\nu}\Box\mathfrak{R} - 2\mathfrak{R}R_{\mu\nu} + \frac{1}{2}g_{\mu\nu}\mathfrak{R}^2, \tag{139}$$

and d_i the remaining renormalization freedom.[17]

We want to express $\langle : \mathbf{T} : \rangle[e_0, e_1]$ and $\langle : \mathbf{T} : \rangle[e_1, e_1]$ on a characteristic surface C_t in terms of the regularized boundary two-point function w_t, going through the same procedure as for the Wick squares, we find that

$$\begin{aligned}\mathbf{T}[e_0, e_1] =& \frac{1}{8\pi^2}\Bigg(\frac{1}{2r^2}\exp(-2\beta)\left(\frac{1}{2}\vec{\nabla}^2_\Omega[w_t] - [\vec{\nabla}^2_\Omega w_t]\right) + \frac{1}{2}m^2[w_t] \\ &+ e_0^\mu e_1^\nu \xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box\right][w_t]\Bigg) \\ &+ \mathbf{Q_T}[e_0, e_1],\end{aligned} \tag{140}$$

and

$$\begin{aligned}\mathbf{T}[e_1, e_1] =& \frac{1}{8\pi^2}\Bigg(\exp(-4\beta)\left(\frac{1}{2}\partial_r^2[w_t] - [\partial_r^2 w_t]\right) \\ &+ e_1^\mu e_1^\nu \xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box\right][w_t]\Bigg) \\ &+ \mathbf{Q_T}[e_1, e_1],\end{aligned} \tag{141}$$

where

$$\begin{aligned}\mathbf{Q_T}[e_0, e_1] =& -\frac{1}{2r^2}\exp(-2\beta)Q_{\Phi\Delta_\Omega\Phi} + \frac{1}{2}m^2 Q_{\Phi^2} \\ &+ e_0^\mu e_1^\nu \xi\left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box\right]Q_{\Phi^2} \\ &- D + r.f.,\end{aligned} \tag{142}$$

[17] When $\langle : \mathbf{T} : \rangle$ is used as a source in the semi-classical Einstein equations, one can absorb d_3 and d_4 into a redefinition of Newtons constant and an introduction of the Cosmological constant respectively. See Ref. [27].

and

$$\mathbf{Q_T}[e_1, e_1] = \exp(-4\beta) \left(\frac{1}{2}\partial_r^2 Q_{\Phi^2} - Q_{\Phi\partial_r^2\Phi}\right) + e_1^\mu e_1^\nu \xi \left[R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathfrak{R} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box\right] Q_{\Phi^2} + r.f., \tag{143}$$

with $r.f.$ the residual renormalization freedom. Generally the correction terms $\mathbf{Q_T}[e_0, e_1]$ and $\mathbf{Q_T}[e_1, e_1]$ contain second or higher order derivatives in t of the functions α and β. However, in the case of conformal coupling ($\xi = \frac{1}{6}$), we can actually choose our renormalization freedom such that these terms do not appear. Setting

$$d_2 = \frac{1}{17280\pi^2}, \tag{144}$$

and using the tensor $\mathbf{H}$, defined in Ref. [32] as

$$H_{\mu\nu} = -R_\mu{}^\alpha R_{\alpha\nu} + \frac{2}{3}\mathfrak{R}R_{\mu\nu} + \frac{1}{2}R^{\alpha\beta}R_{\alpha\beta}g_{\mu\nu} - \frac{1}{4}\mathfrak{R}^2 g_{\mu\nu}, \tag{145}$$

we find

$$\begin{aligned}\mathbf{Q_T}[e_0, e_1] =& \frac{1}{2880\pi^2}\mathbf{H}[e_0, e_1] - \frac{m^2}{96\pi^2}\mathbf{G}[e_0, e_1] + \frac{m^4}{32\pi^2}\mathbf{g}[e_0, e_1] \\ &+ \frac{(d\Omega^2)^{\mu\nu}}{1920\pi^2 R^2}\left[\frac{1}{3}\left(-6\nabla^\alpha\nabla^\beta C_{\alpha\mu\beta\nu} + (4\nabla_\mu\nabla_\nu - 3R_{\mu\nu})\mathbf{C}[e_0, e_1, e_0, e_1]\right)\right. \\ &\qquad + g_{\mu\nu}\left(\frac{8}{3}\Box + \frac{1}{6}\mathfrak{R} - 18\mathbf{C}[e_0, e_1, e_0, e_1]\right. \\ &\qquad \left.\left. + 5\mathbf{R}[e_0, e_1, e_0, e_1] - 6R^{-2}\right)\mathbf{C}[e_0, e_1, e_0, e_1]\right] \\ &+ r.f.,\end{aligned} \tag{146}$$

and

$$\begin{aligned}\mathbf{Q_T}[e_1, e_1] =& \frac{1}{2880\pi^2}\mathbf{H}[e_1, e_1] - \frac{m^2}{96\pi^2}\mathbf{R}[e_1, e_1] \\ &+ \frac{1}{2880\pi^2}e_1^\mu e_1^\nu\Big(- 6\nabla^\alpha\nabla^\beta C_{\alpha\mu\beta\nu} + 4\nabla_\mu\nabla_\nu\mathbf{C}[e_0, e_1, e_0, e_1] \\ &\qquad - (3R_{\mu\nu} + 9(\nabla_\alpha e_1^\alpha)^2(e_0)_\mu(e_0)_\nu)\mathbf{C}[e_0, e_1, e_0, e_1]\Big) \\ &+ r.f..\end{aligned} \tag{147}$$

As mentioned above, if the state on which we are evaluating the stress-energy tensor is rotationally invariant, we can calculate all other components of the stress-tensor from these two. Given conformal coupling, we can use the fact that for this renormalization choice, the trace of the stress-energy tensor (involving the trace anomaly as found in Ref. [33]) can be calculated to be

$$\langle : T : \rangle = g^{\mu\nu}\langle : T_{\mu\nu} : \rangle = -m^2\langle : \Phi^2 : \rangle + \frac{m^4}{32\pi^2} + \frac{1}{2880\pi^2}\left(R^{\alpha\beta\gamma\delta}R_{\alpha\beta\gamma\delta} - R^{\alpha\beta}R_{\alpha\beta}\right). \tag{148}$$

This gives us

$$\langle : \mathbf{T}[e_2, e_2] : \rangle = \langle : \mathbf{T}[e_3, e_3] : \rangle = \frac{1}{2}\left(g^{\mu\nu}\langle : T_{\mu\nu} : \rangle + 2\langle : \mathbf{T}[e_0, e_1] : \rangle\right). \tag{149}$$

To find $\langle : \mathbf{T}[e_0, e_0] : \rangle$ we use the divergenceless of $\langle : \mathbf{T} : \rangle$. In particular we use

$$\langle : T_{\mu\nu} : \rangle \nabla^\mu e_0^\nu = \eta^{ab}\nabla_\mu e_a^\mu \langle : \mathbf{T}[e_b, e_0] : \rangle, \tag{150}$$

where we note that

$$\nabla^{(\mu}{e_0}^{\nu)} = \frac{1}{2r}\left(\exp(2\alpha)\left(r\partial_r\alpha - 1\right){e_0}^{(\mu}{e_1}^{\nu)} - \left(\exp(2\alpha)\left(r\partial_r\beta + 1\right) - 2r\partial_t\beta\right)g^{\mu\nu}\right). \tag{151}$$

This allows us to write down

$$\begin{aligned}\partial_r R^2\langle : \mathbf{T}[e_0, e_0] : \rangle = &- R^2\exp(2\beta)\langle : T_{\mu\nu} : \rangle\nabla^{(\mu}{e_0}^{\nu)} \\ &- \partial_t R^2\exp(2\beta)\langle : \mathbf{T}[e_0, e_1] : \rangle \\ &+ \frac{1}{2}\partial_r R^2\exp(2(\alpha+\beta))\langle : \mathbf{T}[e_0, e_1] : \rangle,\end{aligned} \tag{152}$$

So indeed given that we know $\langle : \mathbf{T}[e_0, e_1] : \rangle$ and $\langle : T : \rangle$ on some time interval, we can determine $\langle : \mathbf{T}[e_0, e_0] : \rangle$ (given that our geometry and state is sufficiently regular at $r = 0$). Note that in the massless conformally flat limit we recover exactly the results from Ref. [32].

5 An application: the response of non-linear observables to gravitational collapse

As was first shown in Ref. [34], a black hole background gives rise to a particle production process for the quantum fields propagating on it. That is to say, for an asymptotically flat astrophysical black hole space-time, given that near asymptotic past null infinity the field is in the vacuum state (see Ref. [5] where this notion is made precise), an observer far away from the black hole will at late times observe thermal radiation coming from the direction of the black hole.[18] Such outgoing radiation carries away energy to infinity and, under some assumptions (see e.g. Ref. [37]), one can show that if the black hole background satisfies the semi-classical Einstein equations, this means that the black hole effectively loses mass, i.e. it has a shrinking apparent horizon. This effect is known as *black hole evaporation*. If this effect continues until the horizon hits a black hole singularity, this gives rise to a number of conceptual issues that are often referred to as the *information loss paradox*.[19] It should be noted that calculations on Hawking radiation observed at asymptotic infinity are of limited use when it comes to understanding the dynamics of semi-classical black hole formation and evaporation. One would like to know *where and when* Hawking radiation (which includes both the late time thermal radiation as well as all other modes that one could observe at asymptotic future null infinity) is produced. Certainly its origin can be traced back to the gravitational collapse that ought to have formed a black hole, but in order to understand what the local backreaction of Hawking radiation is on the geometry as a whole, one needs to be able to locally calculate the stress-energy tensor of the quantum field, especially around the

[18] As is well known, for an eventually stationary black hole, this late time radiation should be at the Hawking temperature

$$T_H = \frac{\kappa}{2\pi}, \tag{153}$$

with κ the surface gravity at the event horizon. In the context of black hole thermodynamics this temperature is associated to the black hole itself (see Ref. [27]), and in fact one can assign a similar temperature to any system with a bifurcate Killing horizon (see Ref. [2]). In the case of the particle creation process mentioned above, the thermality of the radiation at late times can be related to the scaling limit of Hadamard states near the event-horizon of the black hole via a gravitation redshift effect (see Ref. [35] where this is made precise). In fact, even for black holes that are not asymptotically static, one can generalise these ideas with respect to the scaling limit near the apparent horizon of a black hole (see Ref. [36]). As a consequence of these scaling limit arguments, one sees that the thermal behaviour is universal for any initial state, i.e. not just the asymptotic vacuum state, as long as it is Hadamard.

[19] Information loss in this case means that for quantum fields on space-times with fully evaporating black holes, one expects that a final state (i.e. the state near future asymptotic infinity) has less information content (i.e. is less pure) than the initial state. This is at odds with the often held view that a fundamental theory of nature should be unitary and hence information loss ought not to occur in a theory underlying semi-classical gravity, i.e. quantum gravity (see Ref. [38]). This stance is not uncontroversial, as one can also take the point of view that information loss is just *part of life* (see Ref. [39]). These conceptual points aside, space-times of this sort also lead to more technical problems, as it is unclear if quantum field theories on space-times with such causal defects as the naked singularity produced at the end of evaporation even admit sensible states in the first place (see Ref. [40]).

collapsing body. Analytic calculations are available in two-dimensional toy models (see Ref. [41]), but there is no guarantee that these results carry over to more realistic (four dimensional) models. We should also take note of numerical approaches to calculating the expectation values of locally covariant non-linear observables for quantum fields on black hole space-times, such as the methods described in Ref. [42] and in Ref. [43], as well as a lattice approach to semi-classical gravity recently proposed in Ref. [44]. However, in the former two approaches a full analysis of the stress-tensor of a quantum field on a dynamical black hole has, to the knowledge of the authors, not yet been carried out to satisfactory degree, while in the latter approach we feel some additional work is required to ensure that the stress tensor calculated using this method is (approximately) locally covariant in the relevant regimes.

As an application of our characteristic approach to Hadamard states and the calculation of non-linear observables, we shall demonstrate how one can use these methods to calculate non-linear observables of Hawking radiation produced in a simple collapse model as an expansion in the black hole mass. In particular, we shall look at the response of the wick square $:\Phi^2:$ for a massless scalar field in the past asymptotic vacuum state, to the collapse of a thin shell of null dust. We shall also comment on how these methods can be generalized to calculate more involved non-linear observables on arbitrary (spherically symmetric) gravitational collapse space-times, though explicit calculations on these we shall leave for a future publication. Here it should be noted that, as the space-time associated with null shell collapse is not smooth and hence one has to be careful when applying results developed for smooth space-times. Nevertheless, we deem these calculations to be a promising starting point of an investigation to gain a better understanding of semi-classical black hole formation and evaporation.

We consider a massless scalar field $\Phi : \mathcal{D}(M) \to \mathcal{A}(M)$, with M a black hole space-time formed by collapsing null dust with a Schwarzschild radius R_s.[20] Such a space-time is described by the ingoing Vaidya metric

$$\mathrm{d}s^2 = -\left(1 - \frac{\vartheta(t) R_s}{r}\right) \mathrm{d}v^2 + 2dRdv + R^2 \mathrm{d}\Omega^2, \tag{154}$$

[20]Note that since the Ricci scalar of a Vaidya space-time vanishes, the dynamics of the theory and the expectation values of wick squares evaluated for the past asymptotic vacuum state are independent of ξ. In principle one could also consider a massive theory, however for such a quantum field the past asymptotic vacuum state has a more complicated form (see Sec. 3.4), and hence we shall not consider that state here.

where ϑ is the Heaviside step function (see Ref. [45]).[21] We would like to bring this metric in quasi-conformal form (i.e. in the form of eq. (4)), which are in particular outgoing coordinates. Typically, it may not be possible to cover the full space-time with a quasi-conformal globally hyperbolic coordinate patch, but in this case we find two distinct patches that lend themselves for answering different questions regarding the Hawking effect. Patch I covers the entire black hole exterior, and the coordinates are uniquely fixed by matching them to outgoing Vaidya coordinates in the post collapse region. This patch is well-suited to re-derive the original results due to Hawking for this collapse model, namely the radiation spectrum at future asymptotic infinity. Patch II covers a neighbourhood of the collapsing shell, inculding the path of the shell inside the black hole interior, and is therefore more suited to gather information about non-linear observables during gravitational collapse.

5.1 Constructing quasi-conformal coordinates

The first step in constructing the quasi-conformal coordinates, is to go to double-null coordinates. This entails solving the equation

$$\partial_v R(v,u) = \frac{1}{2}\left(1 - \frac{\theta(v) R_s}{R(v,u)}\right), \tag{155}$$

where R is the radial coordinate of the Vaidya space-time, such that $4\pi R^2$ measures the area of a 2-sphere centered around the axis of symmetry. For patch I, we demand that

$$\lim_{v\to\infty} \frac{2R_I(v,u)}{v-u} = 1. \tag{156}$$

This gives a solution

$$\begin{aligned} R_I(v,u) =& \vartheta(v)\left(R_s + R_s W\left(\exp\left(\frac{v-u}{2R_S} - 1\right)\right)\right) \\ &+ \vartheta(-v)\left(\frac{v}{2} + R_s + R_s W\left(\exp\left(\frac{-u}{2R_S} - 1\right)\right)\right). \end{aligned} \tag{157}$$

Here W is the prime branch of the Lambert W-function (see Ref. [47]) and u has as domain the full real number line. The metric now takes the form

$$\mathrm{d}s^2 = 2\frac{\partial R(v,u)}{\partial u}\mathrm{d}u\mathrm{d}v + R(v,u)^2\mathrm{d}\Omega^2. \tag{158}$$

[21]This set-up is also considered in Ref. [46], where a mode-sum approach to evaluation of the stress-tensor is proposed.

To transform to quasi-conformal coordinates, we leave u unchanged, but define the coordinate r by the relation

$$\frac{\partial r_I^{-1}}{\partial v} = -\frac{\partial R_I^{-1}}{\partial u}. \tag{159}$$

For this choice of coordinates, a solution to the relation above, with boundary condition

$$\lim_{v\to\infty} r_I(v,u)^{-1} = 0, \tag{160}$$

yields a well defined (non-negative) function that is strictly increasing in v for the full black hole exterior (and hence one can inverse this function to get a well defined r coordinate on the full exterior). This means we can define the quasi-conformal coordinate patch I on the full black hole exterior, as drawn in Figure II.2. In particular, one finds

$$r_I(v,u) = \vartheta(v)R_I(v,u) + \vartheta(-v)\frac{R_I(0,u)^2(v+2R_I(0,u))}{2R_I(0,u)^2 + R_S v}. \tag{161}$$

Using (u, r, Ω) coordinates, the metric takes quasi-conformal form, with

$$\begin{aligned}\exp(2\alpha_I(u,r)) =& \vartheta(r - R_I(0,u))\left(1 - \frac{R_S}{r}\right) \\ &+ \vartheta(R_I(0,u) - r)\frac{R_I(0,u)^3 - 3rR_I(0,u)R_S + 2r^2 R_S}{R_I(0,u)^3},\end{aligned} \tag{162}$$

and

$$\exp(\beta_I(u,r)) = 1 - \vartheta(R_I(0,u) - r)R_S\frac{R_I(0,u) - r}{R_I(0,u)^2 - rR_S}. \tag{163}$$

Using the quasi-conformal metric defined by functions α_I and β_I as above to calculate $\kappa_u^{(0)}$ from equation (76), one finds that for $r < R_I(0,u) < r'$

$$\kappa_{u,I}^{(0)}(r,r') = R_S\frac{(r+r')(R_I(0,u)^3 - 3rr'R_I(0,u)) + 4r^2r'^2}{4rr'(r'-r)^3R_I(0,u)^3}, \tag{164}$$

and that it is zero for $r, r' < R_I(0,u)$ and $r, r' > R_I(0,u)$. This function plays a role in the source term for $\tilde{\lambda}_u$ (as defined in (77)), in particular

$$(\partial_t\partial_r\partial_{r'} - K_t\partial_{r'} - K_t'\partial_r)RR'\tilde{\lambda}_u(r,\Omega;r',\Omega') = -2\pi\kappa_u^{(0)}(r,r')\delta(\Omega,\Omega'). \tag{165}$$

This relation is admittedly somewhat formal, as it only really holds when both sides of the equations are smeared with $\tilde{S}_{s.c.}(C_u)$ functions (as defined

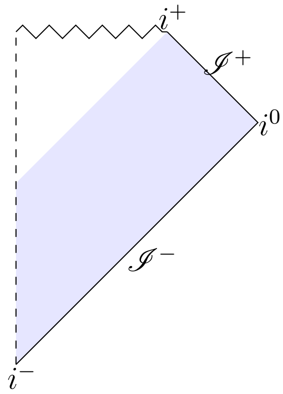

Figure II.2: A Penrose diagram of the space-time with the Vaidya metric of eq. (154) with the domain of coordinate patch I as shaded region

in Sec. 2.3).[22] Nevertheless we can loosely think of $\kappa_u^{(0)}$ as sourcing the 'particle production' for our quantum field living on a gravitational collapse space-time. This really highlights the fact that the produced radiation originates near the collapsing body, as opposed to near the horizon, as is sometimes suggested.[23] As discussed in detail in [35], the presence of a Killing horizon in the post collapse region implies that the radiation observed at $\mathscr{I}^+$ asymptotes towards a thermal spectrum, simply due to the universal nature of a black hole geometry near such an horizon. Verifying the thermality of the radiation produced in this particular collapse process, requires calculating the asymptotic spectrum, which is a calculation we shall leave for another time. What we will note is that the fact that the observed radiation asymptotes to

[22]Note in particular that the asymptotic mode functions typically used to calculate the spectrum of the radiation produced in gravitational collapse, as observed by an observer near $\mathscr{I}^+$, cannot be embedded into $\tilde{S}_{s.c.}(C_u)$ via (R-weighted) restriction to C_u. Not only because these mode functions are not spatially compact, but also because mode function typically diverge near the tip of C_u. This means in particular that the relation above cannot be expected to hold when smeared with mode-functions, in fact the right hand side will typically be divergent. Therefore, one cannot use this relation directly to calculate the spectrum of the produced radiation. This can be mended by going to a higher order of Hadamard subtraction, for which the resulting source term (given by eq. (86) cut off at finite n) is more well-behaved near $r = 0$ and hence can be integrated with a larger class of functions.

[23]It is slightly suggestive to speak of a region of origin of this radiation in the first place. As can be seen from the support of $\kappa_u^{(0)}$, the correlations of the two-point functions between past and post collapse regions (i.e. the regions separated by $r = R_I(0, u)$) are what is primarily sourced by $\kappa_u^{(0)}$. Of course these correlations then propagate to asymptotic infinity, where they then read as radiation coming from the direction of the collapsing body.

a steady state (such as thermal radiation), can already be seen directly from $\kappa_u^{(0)}$, as for $r < R_I(0,u) < r'$ this function asymptotes to

$$\lim_{u\to\infty} \kappa_u^{(0)}(r,r') = \frac{(r+r')(R_S^3 - 3rr'R_S) + 4r^2r'^2}{4rr'(r'-r)^3R_S^2}. \tag{166}$$

Shifting away from patch I, we will focus with more detail on coordinate patch II. We construct this patch by solving (155), where we demand that for $v < 0$

$$R_{II}(v,u) = \frac{v-u}{2}. \tag{167}$$

This gives for $v > 0$ that

$$R_{II}(v,u) = R_S + R_S W\left(-\frac{u+2R_S}{2RS}\exp\Big(\frac{v-u-2R_S}{2R_S}\Big)\right). \tag{168}$$

Here the domain of u is $(-\infty, 0)$. Similarly to the null coordinates used to construct patch I, the function R_{II} above can be used to construct null coordinates on the black hole geometry. However, in this instance these null coordinates cover the full space-time, where the metric again takes the form

$$\mathrm{d}s^2 = 2\frac{\partial R_{II}(v,u)}{\partial u}\mathrm{d}u\mathrm{d}v + R_{II}(v,u)^2\mathrm{d}\Omega^2. \tag{169}$$

Using once more the relation

$$\frac{\partial r_{II}^{-1}}{\partial v} = -\frac{\partial R_{II}^{-1}}{\partial u}, \tag{170}$$

to define quasi-conformal coordinates (u, r_{II}, Ω), we find that for $u \neq -2R_S$

$$r_{II}(v,u) = \vartheta(-v)\frac{v-u}{2} + \vartheta(v)\frac{-uR_{II}(v,u)(u+2R_S)}{4R_SR_{II}(v,u) - u^2}, \tag{171}$$

while for $u = -2R_S$ this relation can be extended by continuity to

$$r_{II}(v,-2R_S) = \vartheta(-v)\frac{v+2R_S}{2} + \vartheta(v)\frac{R_S}{2-\exp\left(\frac{v}{2R_S}\right)}. \tag{172}$$

It should be noted that r_{II} blows up near the surface

$$R_{II}(v,u) = \frac{u^2}{4R_S}, \tag{173}$$

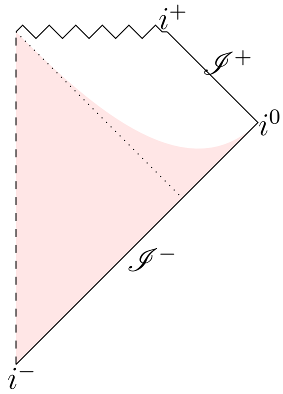

Figure II.3: A Penrose diagram of the space-time with the Vaidya metric of eq. (154) with the domain of coordinate patch II as shaded region, and the dotted line denoting the collapsing shell

hence these quasi-conformal coordinates can only be used to cover the black hole space-time up to this boundary.[24] Luckily, the full trajectory of the collapsing body is contained within the patch where r_{II} is defined. Furthermore, we can calculate the induced metric on this boundary surface, namely

$$\mathrm{d}s^2 = \left(1 - \frac{u}{R_S}\right)\mathrm{d}u^2 + \frac{u^4}{16R_s^2}\mathrm{d}\Omega^2, \tag{174}$$

which in particular means that this (future) boundary is space-like. Therefore, patch II, drawn in Figure II.3, is globally hyperbolic.

On the quasi-conformal coordinate patch II, we can now calculate the metric coefficients to be

$$\exp(2\alpha_{II}) = 1 - \vartheta(2r+u)R_S(2r+u)^2\frac{2R_S(2r+u)-(4r-u)u}{ru^4}, \tag{175}$$

$$\exp(\beta_{II}) = 1 - \vartheta(2r+u)\frac{2R_S(2r+u)}{(u^2+2R_S(2r+u))}. \tag{176}$$

5.2 Calculating Wick squares on a Vaidya space-time

Now that we have found a quasi-conformal coordinate patch surrounding the collapsing shell, we want to give an expression for expectation values locally

[24]Strictly speaking this relation defines this surface for $u \neq -2R_S$, by continuity this relation can then be extended to $u = -2R_S$, i.e. where the surface crosses the horizon, which happens at $v = 2R_S\ln(2)$.

covariant non-linear observables that can be used for explicit calculations. As a proof of concept, we shall restrict our attention to $:\Phi^2:$. We consider the two-point function in the asymptotic past vacuum state. Recalling the discussion of Sec. 4, for a two-point function restricted to C_u of the form

$$\Lambda(u, r, \Omega; u, r', \Omega') = \frac{1}{8\pi^2}\Bigg[\frac{\exp(-\beta - \beta')}{rr'(1-\cos\theta) + \mathrm{i}0^+(r - r' - i0^+)} \\ + v_u^{(0)}(r, r')\ln(RR'(1-\cos\theta)) + w_u^{(0)}(r, \Omega; r', \Omega')\Bigg], \tag{177}$$

with $w_u^{(0)}(r, \Omega; r', \Omega')$ a C^1 function, the expectation value of $:\Phi^2:$ is given by the expression

$$\langle :\Phi^2: \rangle_\Lambda = \frac{1}{8\pi^2} w_u^{(0)}(r, \Omega; r, \Omega) + Q_{\Phi^2}. \tag{178}$$

The covariance correction term can be easily calculated to be

$$Q_{\Phi^2} = \vartheta(2r + u)\frac{R_S(u^2 + 2R_S(2r + u))^3}{48\pi^2 r^3 u^6}. \tag{179}$$

Calculating $w_u^{(0)}(r, \Omega; r, \Omega)$ is a bit more involved. First we establish that for $r < \frac{-u}{2} < r'$

$$\kappa_{u,II}^{(0)}(r, r') = \frac{R_s\left(u^3(r + r') - 12urr'(r + r') - 36r^2r'^3\right)rr'u^3(r' - r)^3}{} \\ + \frac{2R_S^2(2r + u)(2r' + u)(r(2r' + u) + r'(2r + u))}{,} \tag{180}$$

and that $\kappa_{u,II}^{(0)}(r, r') = 0$ for $r, r' < -\frac{u}{2}$ and $r, r' > -\frac{u}{2}$. Using relation (83), we find for $r < \frac{-u}{2} < r'$ that

$$v_{u,II}^{(0)}(r, r') = -\frac{R_S(2r + u)(2r' + u)(u^2 + 2R_S(2r' + u))}{4u^7(r' - r)^3} \\ \times\left(u(u^2 - 2(r + r')u - 12rr') + 2R_s(2r + u)(2r' + u)\right), \tag{181}$$

and also that this function is zero for $r, r' < -\frac{u}{2}$ and $r, r' > -\frac{u}{2}$. We can now write a dynamical equation for $w_u^{(0)}(r, \Omega; r', \Omega')$, namely

$$
\begin{aligned}
\left(\partial_u\partial_r\partial_{r'} + K_u\partial_r + K'_u\partial_{r'}\right) RR' w_u^{(0)} = &- \ln(RR'(1-\cos\theta))\kappa_u^{(1)} \\
&- \frac{1}{2}\Big[\frac{1}{RR'}\partial_u RR'\partial_r\partial_{r'} RR' v_u^{(0)} \\
&+ \partial_u \left((\partial_r R)(\partial_{r'} R') v_u^{(0)} - RR'\partial_r\partial_{r'} v_u^{(0)}\right) \\
&+ \frac{R'}{r'^2}\partial_r R v_u^{(0)} \\
&+ (\partial_{r'} R')\left(\exp(2\beta)\tilde{V} - \partial_r \exp(2\alpha)\partial_r\right) R v_u^{(0)} \\
&- \frac{1}{R}(\partial_r R)\exp(2\alpha)\partial_r\partial_{r'} RR' v_u^{(0)}) \\
&- \partial_r \exp(2\alpha)(\partial_r R)\partial_{r'} R' v_u^{(0)}) \\
&+ (r \leftrightarrow r')\Big] =: S_u^{(0)}(r,\Omega;r',\Omega'). \quad (182)
\end{aligned}
$$

Using the formal integration kernel of the map $\rho_u : \mathcal{D}(M_u) \to \tilde{S}_{s.c.}(C_u)$, given by $\rho_u(r,\Omega;\overline{u},\overline{r},\overline{\Omega})$, we can write down a solution to this equation, provided the initial data $\lim_{u\downarrow-\infty} RR' w_u^{(0)}(r,r') = 0$. That being

$$
\begin{aligned}
w_{u_0}^{(0)}(r_0,\Omega_0;r'_0,\Omega'_0) = 4\int_{-\infty}^{u_0} \mathrm{d}u \int \mathrm{d}r \int \mathrm{d}\Omega \int \mathrm{d}r' \int \mathrm{d}\Omega' \\
\rho_u(r,\Omega;u_0,r_0,\Omega_0)\rho_u(r',\Omega';u_0,r'_0,\Omega'_0) S_u^{(0)}(r,\Omega;r',\Omega').
\end{aligned} \quad (183)
$$

While we cannot bring this expression into closed form, we point out that this equation may be used as the starting point for a numerical calculation of w_u.[25] Alternatively, we may expand this equation in powers of R_S. Clearly in the limit $R_S \to 0$, coordinate patch II reduces to (a patch of) Minkowski space-time. Writing the operator $K_t = K_t^{(0)} + R_S K_t^{(1)}$, with $K_t^{(0)}$ the operator in the Minkowski limit (i.e. for $R_S = 0$) we can write $w_u^{(0)}(r,\Omega;r',\Omega')$ as a formal series

$$
w_u^{(0)}(r,\Omega;r',\Omega') = \sum_{n=0}^{\infty} R_S^n w_{u,n}^{(0)}(r,\Omega;r',\Omega'), \quad (184)
$$

[25] Admittedly, numerical calculations involving retarded propagators on black hole space-times are far from easy to implement, especially as they themselves have non-trivial singular behaviour. See for instance Ref. [48] where this problem is studied on a Schwarzschild background.

where

$$\begin{aligned}
&w^{(0)}_{u_0,0}(r_0,\Omega_0;r_0',\Omega_0') = 4\exp(-\beta(u_0,r_0)-\beta(u_0,r_0'))\\
&\times\int_{-\infty}^{u_0}\mathrm{d}u\int\mathrm{d}r\int\mathrm{d}\Omega\int\mathrm{d}r'\int\mathrm{d}\Omega'\rho_{u,0}(r,\Omega;u_0,r_0,\Omega_0)\rho_{u,0}(r',\Omega';u_0,r_0',\Omega_0')\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\times S^{(0)}_u(r,\Omega;r',\Omega'), \quad (185)
\end{aligned}$$

with $\rho_{u,0}$ the (r-weighted) causal propagator on Minkowski space-time, and

$$\begin{aligned}
&w^{(0)}_{u_0,n+1}(r_0,\Omega_0;r_0',\Omega_0') = -4\exp(-\beta(u_0,r_0)-\beta(u_0,r_0'))\\
&\int_{-\infty}^{u_0}\mathrm{d}u\int\mathrm{d}r\int\mathrm{d}\Omega\int\mathrm{d}r'\int\mathrm{d}\Omega'\rho_{u,0}(r,\Omega;u_0,r_0,\Omega_0)\rho_{u,0}(r',\Omega';u_0,r_0',\Omega_0')\\
&\qquad\qquad\times(K^{(1)}_u\partial_{r'}+K^{(1)'}_u\partial_r)R(u,r)R(u,r')w^{(0)}_{u,n}(r,\Omega;r',\Omega'), \quad (186)
\end{aligned}$$

The terms in this series expansion may be calculated numerically, but in principle they may also be calculated by hand. Here we show how to calculate $w_u(r,\Omega;r,\Omega)$ to lowest order in R_S. We make two observations, firstly that for $u_0 > u$ we have that

$$\begin{aligned}
\rho_{u,0}(r,\Omega;u_0,r_0,\Omega_0) =&\frac{r\delta\left(u_0-u+r_0-r-\sqrt{r^2+r_0^2-2rr_0\cos\theta}\right)}{4\pi(u_0-u+r_0-r)}\\
=&\frac{\delta\left(\cos\theta-1+\frac{(u_0-u)(u_0-u+2(r_0-r))}{2rr_0}\right)}{4\pi r_0}. \qquad (187)
\end{aligned}$$

Secondly, to calculate the contribution due to the logarithmic term in $S^{(0)}_u$, we shall use that for $|x|,|x'|<1$, we can calculate the integral

$$\int_0^{2\pi}\mathrm{d}\phi\ln\left(1-xx'-\cos\phi\sqrt{1-x^2}\sqrt{1-x'^2}\right) = 2\pi\ln\left(\frac{1-xx'+|x-x'|}{2}\right). \qquad (188)$$

This can be verified most easily by expanding the integrand in power series of $\cos\theta$. We can now explicitly work out the coincidence limit of w_u to lowest order in R_S, namely

$$\begin{aligned}
w^{(0)}_{u_0}(r_0,\Omega_0;r_0,\Omega_0) =&4\int_{-\infty}^{u_0}\mathrm{d}u\int\mathrm{d}r\int\mathrm{d}\Omega\int\mathrm{d}r'\int\mathrm{d}\Omega'\\
&\rho_{u,0}(r,\Omega;u_0,r_0,\Omega_0)\rho_{u,0}(r',\Omega';u_0,r_0,\Omega_0)\\
&\times S^{(0)}_u(r,\Omega;r',\Omega')+\mathcal{O}(R_S^2)\\
=&-\vartheta(2r_0+u_0)\frac{R_S}{6r_0^3}+\mathcal{O}(R_S^2), \qquad (189)
\end{aligned}$$

We find that this contribution to $\langle : \Phi^2 : \rangle$ exactly cancels that of the covariance correction term Q_Φ, and hence we find

$$\langle : \Phi^2 : \rangle(u, r) = \mathcal{O}(R_S^2). \tag{190}$$

At this point we do not know if there is a particularly deep reason for this lowest order term to vanish. In similar fashion as what is done in Ref. [41] for the 1+1 dimensional case, one would like to compare this result to recent numerical computations of $\langle : \Phi^2 : \rangle$ in the Unruh state, such as performed in Ref. [49]. However, to properly make such a comparison, such first order calculations as performed above are insufficient. At this point we do not know the rate of convergence of the series expansions for any non-linear observable calculated in this way. Hence, the first order term need by no means be the most dominant, especially not once one evaluates these quantities near or beyond the event horizon. Here it should be especially noted that in our method the expansions are given at fixed dimensionfull coordinates, while if one for instance wants to evaluate $\langle : \Phi^2 : \rangle$ at the Schwarzschild radius, the radial coordinate would also need to be rescaled with respect to R_S. That being said, the functions α and β, from which these expectation values are ultimately calculated, have expansions in R_S that for a fixed value of this expansion parameter have better convergence rates as one approaches the collapsing shell. Therefore we suspect that a similar fact may hold for the expansions of $\langle : \Phi^2 : \rangle$.

Of course the mere expecation value of Φ^2 does not tell us much about the estimated back-reaction of the field onto the geometry, for which we would at least need to calculate the expectation value of the stress-energy tensor. Still, generalizing these methods to calculate the relevant components of the stress-energy tensor do not require so much extra effort. However, for these observables the thin shell collapse model used in this section may not be the most practical, as given the low regularity of this space-time one may expect these observables to diverge near the collapsing shell. Thus, in future work we hope to use the methods developed above to calculate the stress-energy tensor of a quantum field on more realistic (and regular) gravitational collapse space-times, both analytically as well as numerically. We hope that this will give us deeper insight into the back-reaction of quantum fields onto the background geometry during gravitational collapse.

6 Concluding remarks

As far as the authors are concerned, the take-home messages of this paper are the following: for spherically symmetric space-times, the singular part of the Hadamard two-point functions restricted to null cones can be described entirely in terms of particular coordinates adapted to the light-cone and in terms of derivatives of metric components at that cone. Here the amount of time-derivatives (w.r.t. a time-function that has the null cone as a level surface) necessary to write down a characteristic Hadamard parametrix modulo C^{2N+1} is at most $N+1$, where for conformal coupled field this number even reduces to N. While the overall form of the singular structure is by no means surprising, as it can be viewed as a restriction of the usual Hadamard series to the characteristic cone, the fact that this characteristic parametrix can be naturally constructed on the full null cone (provided it can be covered by quasi-conformal coordinates), gives us some novel tools in studying the dynamics of Hadamard states, and how they backreact onto a dynamical background geometry. In particular, we have seen how the characteristic Hadamard parametrix can be used to write down a renormalization scheme for non-linear observables, where the separation between the state-dependent and universal part of the two-point function is made such that, at least for conformally coupled theories, the semi-classical Einstein equations somewhat simplify to a pair of differential equations that are first order in time. Whether this actually means that the semi-classical Einstein equations have solutions for any interesting sets of initial data on some null cone, i.e. whether their Goursat problem is well posed, is a question we hope to answer in the future. For now we will end on the point that the use of the characteristic Hadamard parametrix as a tool to locally covariantly renormalize non-linear observables gives us a way to explicitly calculate the expectation value of such observables as some series expansion. It is hoped that these calculations can also be numerically implemented, yielding a calculation method for observables of quantum fields that, as opposed to more involved methods of calculating locally covariant renormalized observables using numerics, does not involve mode expansions of Hadamard states and Hadamard parametrices.

7 Acknowledgements

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Appendix A. Definitions from microlocal anlysis

In this paper we give recite characterizations of (quasi-free) Hadamard states in terms of their wave front sets. These are objects associated with a distribution that play a central role in microlocal analysis. Here we shall recall the relevant definitions. For a more complete and contextualized overview, see Ref. [50].

We shall first define the notion of a distribution.

Definition 18. *On an open subset $V \subset \mathbb{R}^n$, the set of* distributions $\mathcal{D}'(V)$ *are linear maps $u : \mathcal{D}(V) \to \mathbb{R}$, where $\mathcal{D}(V)$ (real) vector space of compactly supported real-valued smooth functions on V, such that for each compact $K \subset V$ there exists a $C \in \mathbb{R}_{>0}$ and an $N \in \mathbb{N}$ such that*

$$|u(f)| \leq C \sup\{|\partial_{x_1}^{\alpha_1} ... \partial_{x_n}^{\alpha_n} f(x)| : x \in K, \, \alpha_i \in \mathbb{N}, \sum_{i=1}^{n} \alpha_i \leq N\}. \tag{A.191}$$

On an smooth n-manifold M, which has an atlas $(U_i, \phi_i)_{i \in I}$ consisting of an open cover $U_i \subset M$ and homeomorphisms $\phi_i : U_i \to V_i \subset \mathbb{R}^n$ such that for each $i, j \in I$ the map $\phi_i \circ \phi_{i'}^{-1}$ is smooth, a distribution density *$\tilde{u} : \mathcal{D}(M) \to \mathbb{R}$ is a linear map such that for each $i \in I$ one can define a distribution $u_i \in \mathcal{D}'(V_i)$ via*

$$u_i(f) = \tilde{u}(f \circ \phi_i), \tag{A.192}$$

with $f \circ \phi_i \in \mathcal{D}(M)$ defined to be 0 outside U_i.

On a space-time M with metric g, the set of distributions $\mathcal{D}'(M)$ *are the linear maps $u : \mathcal{D}(M) \to \mathbb{R}$ such that $\tilde{u} = \mathrm{dvol}_g u$ is a distribution density. This means that for u_i defined above we now have*

$$u_i(f) = u\left(\left(f\sqrt{|g|}\right) \circ \phi_i\right), \tag{A.193}$$

with $|g|$ the absolute value of the determinant of the metric g in local coordinates defined by ϕ_i.[26]

The space of distributions of compact support, i.e. maps $u \in \mathcal{D}'(M)$ for which there is a compact $K \subset M$ such that for each $f \in \mathcal{D}(M)$ with $\mathrm{supp}(f) \cap K = \emptyset$ *we have* $u(f) = 0$ *(where the smallest K for which this holds*

[26]One can define distributions on a manifold without the use of a smooth density, see Ref. [50, Def. 6.3.3.]. In a setting with a canonical choice of strictly positive smooth density defining the integration measure on a manifold, such as in the case of a Lorentzian space-time, distributions and distribution densities are canonically identified with one another as in the definition above.

defines $\mathrm{supp}(u)$*), are denoted by* $\mathcal{E}'(M)$*.* $u \in \mathcal{E}'(M)$ *can be viewed as a map* $u : \mathcal{E}(M) \to \mathbb{R}$ *via the extension given by*

$$(hu)(f) := u(hf), \tag{A.194}$$

with $h \in \mathcal{D}(M)$ *and* $h(x) = 1$ *for each* $x \in \mathrm{supp}(u)$*.*

To define the wave front set, we introduce the Fourier transform of a compactly supported distribution on $\mathbb{R}^n$.

Definition 19. *Given* $u \in \mathcal{E}(\mathbb{R}^n)$*, we can define the* Fourier *transform* $\hat{u} \in \mathcal{E}(\mathbb{R}^n, \mathbb{C})$ *via*

$$\hat{u}(k) = u(\cos(\langle ., k\rangle) - \mathrm{i}u(\sin(\langle ., k\rangle)), \tag{A.195}$$

where $\langle ., .\rangle$ *is the standard Euclidean inner product on* $\mathbb{R}^n$*.*

That this function is indeed smooth follows from Ref. [50, Thm. 2.1.3.]. We now define the wave front set of a distribution.

Definition 20. *For* $V \subset \mathbb{R}^n$ *open and* $u \in \mathcal{D}(V)$*, the* wave front set $WF(u) \subset V \times (\mathbb{R}^n \setminus \{(0, ..., 0)\}) \cong T^*V \setminus \mathbf{0}$ *is defined by* $(x, k) \notin WF(u)$ *if and only if there is an* $h \in \mathcal{D}(V)$ *with* $h(x) \neq 0$ *and a conic open neighbourhood* $k \in \Gamma \subset \mathbb{R}^n$ *such that for each* $N \in \mathbb{N}_{>0}$ *there is a* $C > 0$ *with for any* $\zeta \in \Gamma$

$$|(\hat{hu})(\zeta)| \leq C(1 + |\zeta|)^{-N}. \tag{A.196}$$

Let M *a space-time of dimension* n *with atlas* $(U_i, \phi_i)_{i \in I}$ *and let* $u \in \mathcal{D}'(M)$*. The set* $WF(u) \subset T^*M \setminus \mathbf{0}$*, with* T^*M *the cotangent bundle and* $\mathbf{0} \cong M \times \{(0, ..., 0)\}$ *the zero bundle, is given by* $(x, k) \in WF(u)$ *iff there is an* $i \in I$ *with* $(x, k) \in T^*U_i$ *such that* $(\phi_i(x), \left(\phi_i^{-1}\right)^* (k)) \in WF(u_i)$*.*

The wave front set of a distribution tells us what operations defined on smooth functions (multiplications, restrictions etc.) can be naturally extended to it (see [50, Ch. 8.2.]). Furthermore, the wave front set plays a crucial role in the propagation of singularities of weak solutions to differential equations (see Ref. [51, Sec. 6.1]).

In this paper we mainly use the wave front set in the context of two-point functions. As described in Sec. 2.3, for a real scalar field on a globally hyperbolic space-time M, a two-point function is given by a map $\Lambda : \mathcal{D}(M)^2 \to \mathbb{C}$ with

$$\Lambda(f, g) = \mu(f \otimes g) + \frac{\mathrm{i}}{2}E(f, g), \tag{A.197}$$

where $\mu \in \mathcal{D}'(M \times M)$ with in particular $\mu(f \otimes f) \geq 0$, $\mu(f \otimes Pg) = \mu(Pf \otimes g) = 0$ and $E(f, g)^2 \leq 4\mu(f, f)\mu(g, g)$. For such bi-distributions, which uniquely extend to distributions on $M \times M$, one often works with the primed wave front set $WF'(\Lambda) \subset (T^*M)^2 \setminus \mathbf{0}^2$, which is defined as

$$(x_1, k_1; x_2, k_2) \in WF'(\Lambda) \iff ((x_1, x_2), (k_1, -k_2)) \in WF(\Lambda) \subset T^*(M \times M) \backslash \mathbf{0}. \tag{A.198}$$

For example, for the commutator function E given by Eq. (28), one has

$$WF'(E) = \{(x_1, k_1; x_2, k_2) \in (T^*M \backslash \mathbf{0})^2 : g^{\mu\nu}(x_i)(k_i)_\mu (k_i)_\nu = 0, \ (x_1, k_1) \sim (x_2, k_2)\} \tag{A.199}$$

where the equivalence relation $\sim$ on null covectors is defined as $(x_1, k_1) \sim (x_2, k_2)$ if there exists a null geodesic $\gamma : \mathbb{R} \to M$ with $a, b \in \mathbb{R}$ such that

$$\gamma(a) = x_1, \ g_{\mu\nu}(x_1)\dot{\gamma}(a)^\mu = (k_1)_\nu, \ \gamma(b) = x_2, \ g_{\mu\nu}(x_2)\dot{\gamma}(b)^\mu = (k_2)_\nu. \tag{A.200}$$

A relevant operation on (primed) wave-front sets of bi-distributions is the following.

Definition 21. *Given Λ a bi-distribution on M,or equivalently $\Lambda \in \mathcal{D}'(M \times M)$, we define*

$${}_MWF'(\Lambda) = \{(x_2, k_2) \in T^*M \backslash \mathbf{0} : (x_1, 0; x_2, k_2) \in WF'(\Lambda) \ \textit{for some} \ x_1 \in M\}, \tag{A.201}$$

and

$$WF'(\Lambda)_M = \{(x_1, k_1) \in T^*M \backslash \mathbf{0} : (x_1, k_1; x_2, 0) \in WF'(\Lambda) \ \textit{for some} \ x_2 \in M\}. \tag{A.202}$$

These objects correspond to the wave front sets of Λ smeared with a single $f \in \mathcal{D}(M)$. In particular, as proven in Ref. [50, Thm. 8.2.12.],

$$WF(\Lambda(f, .)) = -{}_MWF'(\Lambda), \ WF(\Lambda(., f)) = WF'(\Lambda)_M. \tag{A.203}$$

Appendix B. Detailed derivations of formulas

Here we write out the derivations of certain formulas from the main text in some more detail.

B.1 Equation (54)

This relation is somewhat formal, meaning that it may not be well-defined for all distributions, hence one has to verify whether this relation holds for a particular class of distributions at hand. Let us in this case consider a family of functions $\lambda_t \in L_1(C_t^2, \mathrm{d}r\mathrm{d}r'\mathrm{d}\Omega\mathrm{d}\Omega')$ for $t \in \mathbb{R}$ such that $\partial_t\lambda_t \in L_1(C_t^2, \mathrm{d}r\mathrm{d}r'\mathrm{d}\Omega\mathrm{d}\Omega')$. This family generates bi-distributions $\Lambda_t \in \mathcal{D}(M_t \times M_t)$ in the bulk via

$$\Lambda_t(f,g) = \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \lambda_t(r,\Omega;r',\Omega')\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega'). \tag{B.204}$$

We assume that for given $f, g \in \mathcal{D}(M_t)$ there is a $\delta > 0$ such that for $t-\delta < t' < t+\delta$ we have $\Lambda_t(f,g) = \Lambda_{t'}(f,g)$, which means in particular that

$$\frac{\mathrm{d}\Lambda_t(f,g)}{\mathrm{d}t} = 0. \tag{B.205}$$

Let us furthermore assume for each $t' \in (t-\delta, t+\delta)$ there exists a $\tilde{\lambda} \in L_1(C_t^2, \mathrm{d}r\mathrm{d}r'\mathrm{d}\Omega\mathrm{d}\Omega')$ such that $|\lambda_{t'}| \leq \tilde{\lambda}$ almost everywhere on C_t^2. In this case we can use the Leibniz integral rule to derive

$$\begin{aligned}
0 =& \frac{\mathrm{d}}{\mathrm{d}t} \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \lambda_t(r,\Omega;r',\Omega')\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') \\
=& \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \left(\partial_t\lambda_t(r,\Omega;r',\Omega')\right) \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') \\
&+ \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \lambda_t(r,\Omega;r',\Omega') \left(\partial_t\rho_t(f)(r,\Omega)\right) \rho_t(g)(r',\Omega') \\
&+ \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \lambda_t(r,\Omega;r',\Omega')\rho_t(f)(r,\Omega) \left(\partial_t\rho_t(g)(r',\Omega')\right)
\end{aligned}$$

$$
\begin{aligned}
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \, \left(\partial_t \lambda_t(r,\Omega;r',\Omega')\right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \lambda_t(r,\Omega;r',\Omega') \left(\int_r^\infty \mathrm{d}s \, \left(K_t \rho_t(f)\right)(s,\Omega) \right) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \lambda_t(r,\Omega;r',\Omega') \rho_t(f)(r,\Omega) \left(\int_{r'}^\infty \mathrm{d}s \, \left(K_t \rho_t(g)\right)(s,\Omega') \right) \\
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \, \left(\partial_t \lambda_t(r,\Omega;r',\Omega')\right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(\int_0^s \mathrm{d}r \, \lambda_t(r,\Omega;r',\Omega') \right) \left(K_t \rho_t(f)\right)(s,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}s \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(\int_0^s \mathrm{d}r' \, \lambda_t(r,\Omega;r',\Omega') \right) \rho_t(f)(r,\Omega) \left(K_t \rho_t(g)\right)(s,\Omega') \\
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \, \left(\partial_t \lambda_t(r,\Omega;r',\Omega')\right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(\int_0^r \mathrm{d}s \, \lambda_t(s,\Omega;r',\Omega') \right) \left(K_t \rho_t(f)\right)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(\int_0^{r'} \mathrm{d}s \, \lambda_t(r,\Omega;s,\Omega') \right) \rho_t(f)(r,\Omega) \left(K_t \rho_t(g)\right)(r',\Omega') \\
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \, \left(\partial_t \lambda_t(r,\Omega;r',\Omega')\right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(K_t \int_0^r \mathrm{d}s \, \lambda_t(s,\Omega;r',\Omega') \right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega') \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega' \\
&\qquad\qquad \left(K_t' \int_0^{r'} \mathrm{d}s \, \lambda_t(r,\Omega;s,\Omega') \right) \rho_t(f)(r,\Omega) \rho_t(g)(r',\Omega'). \qquad \text{(B.206)}
\end{aligned}
$$

This relation holds for all test functions $f, g \in \mathcal{D}(M_t)$, from Ref. [52] we can conclude that the image of ρ_t is dense in an appropriate Sobolev space on C_t, which allows us to conclude that

$$\partial_t \lambda_t(r,\Omega;r',\Omega') + K_t \int_0^r \mathrm{d}s\, \lambda_t(s,\Omega;r',\Omega') + K'_t \int_0^{r'} \mathrm{d}s\, \lambda_t(r,\Omega;s,\Omega') = 0. \tag{B.207}$$

For the case of Hadamard two-point functions, λ_t will in general not be an L_1 function. That this argument still goes through can be seen in the following derivation.

B.2 Equation (75)

Consider on a general spherically symmetric space-time with metric (4) a family of null boundary two-point functions

$$\lambda_t = -\frac{1}{\pi} \frac{\delta(\Omega,\Omega')}{(r-r'-\mathrm{i}0^+)^2}, \tag{B.208}$$

on C_t defining Hadamard bulk two-point functions Λ_t on M_t via

$$\Lambda_t(f,g) = -\lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)}{(r-r'-\mathrm{i}\varepsilon)^2}. \tag{B.209}$$

We first note that

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t} \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)}{(r-r'-\mathrm{i}\varepsilon)^2} \\
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\dot\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)}{(r-r'-\mathrm{i}\varepsilon)^2} \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\dot\rho_t(g)(r',\Omega)}{(r-r'-\mathrm{i}\varepsilon)^2} \\
&= \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K_t \int_0^r \mathrm{d}s\, \frac{\delta_{S^2}(\Omega,\Omega')}{(s-r'-\mathrm{i}\varepsilon)^2} \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K'_t \int_0^{r'} \mathrm{d}s\, \frac{\delta_{S^2}(\Omega,\Omega')}{(r-s-\mathrm{i}\varepsilon)^2} \\
&= -\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K_t \frac{\delta_{S^2}(\Omega,\Omega')}{(r-r'-\mathrm{i}\varepsilon)} \\
&\quad - \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K_t \frac{\delta_{S^2}(\Omega,\Omega')}{(r'+\mathrm{i}\varepsilon)} \\
&\quad + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K'_t \frac{\delta_{S^2}(\Omega,\Omega')}{(r-r'-\mathrm{i}\varepsilon)} \\
&\quad - \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \int_{S^2} \mathrm{d}\Omega'\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega') K'_t \frac{\delta_{S^2}(\Omega,\Omega')}{(r-\mathrm{i}\varepsilon)}
\end{aligned}$$

$$
\begin{aligned}
=&-\frac{1}{2}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega) \\
&\qquad \frac{\exp(2\beta(t,r))\tilde{V}(t,r) - \exp(2\beta(t,r'))\tilde{V}(t,r')}{(r-r'-\mathrm{i}\varepsilon)} \\
&+\frac{1}{2}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega) \\
&\qquad \Big(2\frac{\exp(2\alpha(t,r)) - \exp(2\alpha(t,r'))}{(r-r'-\mathrm{i}\varepsilon)^3} \\
&\qquad\quad - \frac{(\partial_{r'}\exp(2\alpha(t,r')) + \partial_r \exp(2\alpha(t,r)))}{(r-r'-\mathrm{i}\varepsilon)^2}\Big) \\
&-\frac{1}{2}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)\frac{\exp(2\beta(t,r))\tilde{V}(t,r)}{(r'+\mathrm{i}\varepsilon)} \\
&-\frac{1}{2}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)\frac{\exp(2\beta(t,r'))\tilde{V}(t,r')}{(r-\mathrm{i}\varepsilon)} \\
&-i\varepsilon\frac{1}{2}\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega)}{rr'(r-r'-\mathrm{i}\varepsilon)}\left(\frac{1}{r'+\mathrm{i}\varepsilon} + \frac{1}{r-\mathrm{i}\varepsilon}\right)
\end{aligned}
\tag{B.210}
$$

With some care, one can take the limit $\varepsilon \downarrow 0$ and show that this is uniform in t on a sufficiently small interval. Let us illustrate this for the last line of the equation above. We consider the integral

$$
\begin{aligned}
&\varepsilon\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega)}{(r'+\mathrm{i}\varepsilon)rr'(r-r'-\mathrm{i}\varepsilon)} \\
=&\varepsilon\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega)}{(r'+\mathrm{i}\varepsilon)rr'}\partial_r \ln(r-r'-\mathrm{i}\varepsilon) \\
=&-\varepsilon\int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\lim_{r\downarrow 0}\frac{R}{r}G_c(f)(t,r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega)}{(r'+\mathrm{i}\varepsilon)r'}\ln(-r'-\mathrm{i}\varepsilon) \\
&-\varepsilon\int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\partial_r\frac{R}{r}G_c(f)(t,r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega)}{(r'+\mathrm{i}\varepsilon)r'}\ln(r-r'-\mathrm{i}\varepsilon).
\end{aligned}
\tag{B.211}
$$

Note that $G_c(f)(t,0,\Omega)$ is independent of Ω. Therefore, we can easily see

$$
\int_{S^2} \mathrm{d}\Omega \lim_{r\downarrow 0}\frac{R}{r}G_c(f)(t,r,\Omega)\Delta_\Omega\rho_t(g)(r',\Omega) = 0. \tag{B.212}
$$

Furthermore, both $\partial_r \frac{R}{r}G_c(f)(t,r,\Omega)$ and $\frac{1}{r^2}\Delta_\Omega\frac{R}{r}G_c(g)(t,r,\Omega)$ are continuous function with spatially compact support, which we shall denote by $F \in C^0(M)$

and $G \in C^0(M)$ respectively. Let r_m be such that for $t \in (a,b)$ some interval we have $F(t,r,\Omega) = G(t,r,\Omega) = 0$ for $r > r_m$. We can now estimate

$$
\begin{aligned}
&\varepsilon \left| \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{\rho_t(f)(r,\Omega)\Delta_\Omega \rho_t(g)(r',\Omega)}{(r'+\mathrm{i}\varepsilon)rr'(r-r'-\mathrm{i}\varepsilon)} \right| \\
\leq&\varepsilon \left| \int_0^{r_m} \mathrm{d}r \int_0^{r_m} \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega\, \frac{H(t,r,\Omega)r'^2 G(t,r',\Omega)}{(r'+\mathrm{i}\varepsilon)} \ln(r-r'-\mathrm{i}\varepsilon) \right| \\
\leq&4\pi\varepsilon \sup_{t\in(a,b),\, r,r'<r_m, \Omega\in S^2} |F(t,r,\Omega)G(t,r,\Omega)| \int_0^{r_m} \mathrm{d}r \int_0^{r_m} \mathrm{d}r'\, r' \left|\ln(r-r'-\mathrm{i}\varepsilon)\right| \\
\leq&4\pi\varepsilon \sup_{t\in(a,b),\, r,r'<r_m, \Omega\in S^2} |F(t,r,\Omega)G(t,r,\Omega)| \\
&\qquad\qquad \times \int_0^{r_m} \mathrm{d}r \int_0^{r_m} \mathrm{d}r'\, r' \left(|\ln|r-r'|| + \left|\ln\left(\sqrt{r_m^2+\varepsilon^2}\right)\right| + \pi \right) .
\end{aligned}
\tag{B.213}
$$

We now see that the integral in question indeed converges to 0 as ε tends to 0. In particular, we see this convergence is uniform in t on some finite interval. This uniform convergence can be established for the full integral of Eq. (B.210) using similar arguments. This means in particular that

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t} \lim_{\varepsilon\downarrow 0} \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \frac{\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)}{(r-r'-i\varepsilon)^2} \\
&\qquad\qquad = \lim_{\varepsilon\downarrow 0} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r' \int_{S^2} \mathrm{d}\Omega \frac{\rho_t(f)(r,\Omega)\rho_t(g)(r',\Omega)}{(r-r'-i\varepsilon)^2},
\end{aligned}
\tag{B.214}
$$

and hence we find Eq. (75).

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