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THERMAL EQUILIBRIUM STATES OF A LINEAR SCALAR QUANTUM FIELD IN STATIONARY SPACE–TIMES

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The linear scalar quantum field, propagating in a globally hyperbolic space–time, is a relatively simple physical model that allows us to study many aspects in explicit detail. In this review, we focus on the thermal equilibrium (KMS) states of such a field in a stationary space–time. Our presentation draws on several existing sources and aims to give a unified exposition, while weakening certain technical assumptions. In particular we drop all assumptions on the behavior of the time-like Killing field, which is important for physical applications to the exterior region of a stationary black hole.

Our review includes results on the existence and uniqueness of ground and KMS states, as well as an evaluation of the evidence supporting the KMS-condition as a characterization of thermal equilibrium. We draw attention to the poorly understood behavior of the temperature of the quantum field with respect to locality.

If the space–time is standard static, the analysis can be done more explicitly. For compact Cauchy surfaces we consider Gibbs states and their properties. For general Cauchy surfaces we give a detailed justification of the Wick rotation, including the explicit determination of the Killing time dependence of the quasi-free KMS states.

Keywords: KMS condition; stationary space–times.

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Contents

1. Introduction

For a quantum mechanical system with a Hilbert space $\mathcal{H}$, a thermal equilibrium state can be described by the density matrix for the Gibbs grand canonical ensemble,

$$\rho^{(\beta,\mu)} := Z^{-1} e^{-\beta(H-\mu N)}, \tag{1.1}$$

where H is the Hamiltonian operator of the system, N the particle number operator, β the inverse temperature and μ the chemical potential.[a] Z is a normalization factor, which ensures that the trace $\operatorname{Tr}\rho^{(\beta,\mu)} = 1$. For this to be well defined we need to know that $e^{-\beta(H-\mu N)}$ is a trace-class operator, a condition which can often be established in explicit models, especially when the system is confined to a bounded region of space.

For physical purposes it is of some interest to study thermal equilibrium in much more general situations than for quantum mechanical systems, such as for a quantum field propagating in a given gravitational background field. In these cases one immediately encounters three well known problems: in a general curved space–time there is no clear notion of particle, no clear choice of a Hamiltonian operator and, even if there were, the exponentiated operator in Eq. (1.1) might not be of trace-class. Additional problems arise if one wants to use the technique of Wick rotation,

[a] We work in natural (Planck) units throughout: $c = G = \hbar = k_B = 1$.

which has important computational advantages in the quantum mechanical case, but which requires a preferred choice of a well behaved time coordinate.

In this paper we treat the problems above for the explicit example of a linear scalar quantum field propagating in a globally hyperbolic space–time. We combine results and arguments from several sources into a unified exposition and we take the opportunity to show that some of the technical conditions made in the earlier literature may be dropped or weakened.

It is well known how to formulate a linear scalar quantum field theory in all globally hyperbolic space–times.[1–4] A notion of particle and Hamiltonian can be introduced whenever the space–time is also stationary.[3] We will therefore focus on stationary space–times, in which case the notion of global thermal equilibrium is (in principle) well understood.[5,6] Under suitable positivity assumptions on the field equation we first give a full characterization of all ground states on the Weyl algebra and we describe in detail a uniquely preferred ground state.[7] More precisely, our assumptions are that the field should satisfy the (modified) Klein–Gordon equation

$$-\Box\phi + V\phi = 0$$

with a smooth, real-valued potential V which is stationary and strictly positive everywhere. Unlike Ref. 7 we do not insist that the ground state should have a mass gap, which allows us to drop the restrictions that the norm and the lapse function of the time-like Killing field be suitably bounded away from zero. This is of some importance in certain physical applications, e.g. when the stationary space–time is the exterior region of a stationary black hole.[8,9] In that case the norm of the Killing field may become arbitrarily small.

Gibbs states as in Eq. (1.1) have a certain property, first noticed by Kubo[10] and Martin and Schwinger[11] and now known as the KMS-condition. This property was proposed as a defining characteristic for thermal equilibrium states by Ref. 12, even when the Gibbs state is no longer defined, on the grounds that it survives the thermodynamic (infinite volume) limit under general circumstances for systems in quantum statistical mechanics in Minkowski space–time. Further support for this proposal comes from an investigation of the second law of thermodynamics for general C^*-dynamical systems[13] and from the study of explicit models in quantum statistical mechanics.[14] In addition to its physical context, the KMS-condition has also become important in the abstract theory of operator algebras, where it is related to Tomita's modular theory.[15]

In the case of a standard static space–time (see Sec. 3 for the definition) with a compact Cauchy surface we will see that the Gibbs state of Eq. (1.1) makes sense. In the case of a general stationary space–time we will give a full characterization of all KMS states on the Weyl algebra and we describe uniquely preferred KMS states at any temperature.[6] Unfortunately, the arguments of Ref. 12 concerning the thermodynamic limit fail to work for quantum field theories. This indicates that the behavior of the temperature of a quantum field, with respect to locality, is presently rather poorly understood, even in a space–time with a favorable background geometry. With a view to physical applications, e.g. in cosmology, an improved understanding would be highly desirable. (At this point we would also like to point out that Refs. 16 and 17 have recently proposed a notion of local thermal equilibrium in general curved space–times, but the full merit of this new approach is as yet unclear and a review of these recent developments is beyond the scope of this paper.)

When we study the Wick rotation we will restrict attention to space–times which are standard static. Under these geometric circumstances there is a preferred Killing time coordinate and it is well understood how KMS states can be obtained from a Wick rotation.[5,18] We show that any technical assumptions are automatically verified for the systems under consideration. After complexifying the Killing time coordinate we obtain an associated Riemannian manifold and we compactify the imaginary time coordinate to a circle of radius R. We then show that there exists a uniquely distinguished Euclidean Green's function, which can be analytically continued back to the Lorentzian space–time. We will find the explicit Killing time dependence of this Green's function and on the Lorentzian side we recover the two-point distribution of the preferred KMS state with inverse temperature $\beta = 2\pi R$.

The contents of this paper are organized as follows. Section 2 considers some basic features of thermal equilibrium states in an abstract, algebraic setting. The main aim is to elucidate the structure of the spaces of all ground and KMS states on the Weyl algebra under minimal assumptions. Section 3 provides a review of recent geometric results on stationary, globally hyperbolic space–times and the subclass of standard static ones. In addition, it introduces the space–time complexification procedure needed to perform the Wick rotation. After these algebraic and geometric preliminaries we describe in Sec. 4 the linear scalar field under consideration, with an emphasis on those results that depend on the presence of the time-like Killing field. This section also contains a discussion of the two-point distributions of thermal equilibrium states. Section 5 considers the space of ground states and the GNS-representation of the uniquely preferred ground state. It also includes a discussion of the renormalized stress-energy–momentum tensor. Section 6 considers thermal equilibrium states at nonzero temperature, from several perspectives. It contains existence results of Gibbs states, under suitable assumptions, and it discusses the motivations to use the KMS-condition to characterize thermal equilibrium. Furthermore, it characterizes all KMS states, including a uniquely preferred one, and in the static case it provides a rigorous justification of the Wick rotation. A number of useful results from functional analysis, needed for Secs. 2, 4 and 6, are collected in the Appendix, so as not to hamper the flow of the presentation. These results concern strictly positive operators and the relation between operators in Hilbert spaces and distributions.

2. Equilibrium States in Algebraic Dynamical Systems

Much of the structure of dynamical systems can be conveniently described in an abstract algebraic setting, which subsumes a great variety of physical applications.

In this section we provide a brief overview of a number of notions and results relating to equilibrium states for such systems and some more specialized results pertaining to Weyl C^*-algebras. (For a detailed treatment of Weyl C^*-algebras we refer to Ref. 19 and references therein.)

Note that we generally do not assume any continuity of the time evolution, so our results must remain more limited than those for C^*-dynamical systems or W^*-dynamical systems.[14,20] This is in line with our physical applications later on, where we will consider the Weyl C^*-algebra of certain pre-symplectic spaces. As it turns out, for these systems the time evolution will not be norm continuous in the given algebra, but there will be continuity at the level of the symplectic space. To accommodate for such situations, the results in this section will only make *ad hoc* continuity assumptions in suitable representations.

2.1. *Algebraic dynamical systems and equilibrium states*

We begin with the following basic definition:

Definition 2.1. An *algebraic dynamical system* $(\mathfrak{A}, \alpha_t)$ consists of a *-algebra $\mathfrak{A}$ with unit I, together with a one-parameter group of *-isomorphisms α_t on $\mathfrak{A}$.

The algebra $\mathfrak{A}$ is interpreted as the algebra of observables and α_t describes the time evolution. A state ω on $\mathfrak{A}$ is a linear functional $\omega : \mathfrak{A} \to \mathbb{C}$ which is normalized, $\omega(I) = 1$, and positive, $\omega(A^*A) \geq 0$ for all $A \in \mathfrak{A}$. Every state gives rise to a unique (up to unitary equivalence) GNS-triple[14] $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$, where $\mathcal{H}_\omega$ is a Hilbert space and π_ω is a representation of $\mathfrak{A}$ on $\mathcal{H}_\omega$, in general by unbounded operators, such that the vector Ω_ω is cyclic for $\pi_\omega(\mathfrak{A})$, i.e. $\overline{\pi_\omega(\mathfrak{A})\Omega_\omega} = \mathcal{H}_\omega$ and $\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle$. We will denote the space of all states on $\mathfrak{A}$ by $\mathscr{S}(\mathfrak{A})$. It is a convex set in the (algebraic) dual space $\mathfrak{A}'$, which is closed in the weak*-topology. We will call a state pure if for any decomposition $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ with $\omega_1, \omega_2 \in \mathscr{S}(\mathfrak{A})$ and $0 < \lambda < 1$ we must have $\omega_1 = \omega_2 = \omega$.

For dynamical systems, the following class of states are of special interest:

Definition 2.2. An *equilibrium state* ω for an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ is a state ω on $\mathfrak{A}$ such that $\alpha_t^*\omega := \omega \circ \alpha_t = \omega$, for all $t \in \mathbb{R}$. We denote the space of all equilibrium states by $\mathscr{G}(\mathfrak{A})$ (suppressing the dependence on α_t).

Note that $\mathscr{G}(\mathfrak{A})$ is a closed convex subset of $\mathscr{S}(\mathfrak{A})$. In the GNS-representation space of an equilibrium state ω the time evolution α_t is implemented by a unitary group U_t via

$$\pi_\omega(\alpha_t(A)) = U_t \pi_\omega(A) U_t^{-1}, \quad A \in \mathfrak{A}.$$

The group U_t is uniquely determined by the additional condition that $U_t\Omega_\omega = \Omega_\omega$ (cf. Ref. 14, Corollary 2.3.17). If the group U_t is strongly continuous, it has a self-adjoint generator by Stone's Theorem (Ref. 21, Theorem VIII.8), so we may write $U_t = e^{ith}$, where the self-adjoint operator h is called the Hamiltonian.

2.1.1. *Ground states*

Definition 2.3. A *ground state* ω on an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ is an equilibrium state for which $U_t = e^{ith}$ is strongly continuous and the Hamiltonian h satisfies $h \geq 0$. We denote the space of all ground states by $\mathscr{G}^0(\mathfrak{A})$.

A ground state ω is called *nondegenerate* when the eigenspace of h with eigenvalue 0 is one-dimensional, i.e. $h\psi = 0$ implies $\psi = \lambda\Omega_\omega$ for some $\lambda \in \mathbb{C}$.

A ground state ω is called *extremal* if for any decomposition $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ with ω_1, $\omega_2 \in \mathscr{G}^0(\mathfrak{A})$ and $0 < \lambda < 1$ we must have $\omega_1 = \omega_2 = \omega$.

Note that pure ground states are always extremal. Furthermore, we have the following result, which is essentially due to Borchers:[22]

Theorem 2.1. *A nondegenerate ground state ω on an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ with $\mathfrak{A}$ a C^*-algebra is pure.*

Proof. The strongly continuous unitary group U_t on $\mathcal{H}_\omega$ defines a group of automorphisms on the von Neumann algebra $\mathfrak{R} := \pi_\omega(\mathfrak{A})''$. (A $'$ denotes the commutant of an algebra and $''$ the double commutant.[15]) The result of Ref. 22 is that $U_t \in \mathfrak{R}$, for all $t \in \mathbb{R}$. Now any unit vector ψ of the form $\psi = X\Omega_\omega$ with $X \in \mathfrak{R}'$ satisfies $h\psi = Xh\Omega_\omega = 0$. Because Ω_ω is cyclic for $\mathfrak{R}$, it is separating for $\mathfrak{R}'$, so $\psi = \lambda\Omega_\omega$ if and only if $X = \lambda I$. Hence if ω is nondegenerate, then $\mathfrak{R}' = \mathbb{C}I$, which means that ω is pure (Ref. 15, Theorem 10.2.3). $\square$

In the case that $\mathfrak{A}$ is commutative, ground states have a special property which is worth singling out. The proof involves analytic continuation arguments which are typical for the study of ground and KMS states:

Lemma 2.1. *Let ω be a state on an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ with $\mathfrak{A}$ a commutative *-algebra. Then the following statements are equivalent*:

(i) *ω is a ground state,*
(ii) *$\omega(A\alpha_t(B)) = \omega(AB)$ for all A, $B \in \mathfrak{A}$ and $t \in \mathbb{R}$,*
(iii) *ω is an equilibrium state with $U_t = I$ for all $t \in \mathbb{R}$, in the GNS-representation of ω.*

Proof. Suppose that ω is a ground state. For arbitrarily given A, $B \in \mathfrak{A}$ we consider the function $f(t) := \omega(A\alpha_t(B)) = \omega(\alpha_t(B)A)$. Because $h \geq 0$ (by definition of ground states) we may use Lemma A.8 to define a bounded, continuous function $F_+(z)$ on the upper half plane $\{z := t + i\tau \mid \tau \geq 0\}$ by

$$F_+(z) := \left\langle \pi_\omega(A^*)\Omega_\omega, e^{izh}\pi_\omega(B)\Omega_\omega \right\rangle,$$

which is holomorphic on $\tau > 0$ and satisfies $F_+(t) = f(t)$ for $\tau = 0$. Similarly we can define a bounded continuous function $F_-(z)$ on the lower half plane by

$$F_-(z) := \left\langle \pi_\omega(B^*)\Omega_\omega, e^{-izh}\pi_\omega(A)\Omega_\omega \right\rangle,$$

which is holomorphic for $\tau < 0$ and which again satisfies $F_-(t) = f(t)$, for $\tau = 0$. It follows from the Edge of the Wedge Theorem[23] that there is an entire holomorphic function F which extends both F_+ and F_-. Since F must be bounded as well it is constant by Liouville's Theorem.[23] Restricting to $\tau = 0$ we find $f(t) = f(0)$, i.e. $\omega(A\alpha_t(B)) = \omega(AB)$.

Now suppose that the second item holds for ω. Then ω is an equilibrium state (taking $A = I$) and using the group properties of α_t one easily shows that $\omega(A\alpha_t(B)C) = \omega(ABC)$, for all $t \in \mathbb{R}$ and A, B, $C \in \mathfrak{A}$. This implies that $\pi_\omega(\alpha_t(B)) = \pi_\omega(B)$ and hence that $U_t = I$ for all $t \in \mathbb{R}$. Finally, $U_t = I$ implies $h = 0$, so ω is a ground state. $\square$

Lemma 2.1 allows us to give a nice description of all ground and equilibrium states on those algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ for which $\mathfrak{A}$ is a commutative C^*-algebra. For this we make use of the classic structure theorem for commutative C^*-algebras (cf. Ref. 15, Theorem 4.4.3), which tells us that there is a compact Hausdorff space X, unique up to homeomorphism, and a *-isomorphism $\alpha : \mathfrak{A} \to C(X)$, where $C(X)$ is the C^*-algebra of continuous, complex-valued functions on X in the suppremum norm. The one-parameter group of *-isomorphisms $\beta_t := \alpha \circ \alpha_t \circ \alpha^{-1}$ on $C(X)$ is then given by $\beta_t(F) = \Psi_t^* F$, where Ψ_t is a (uniquely determined) one-parameter group of homeomorphisms of X. We define the set of fixed points $X_0 := \{x \in X \mid \Psi_t(x) = x \text{ for all } t \in \mathbb{R}\}$, which is closed in X and hence compact.

Theorem 2.2. *Using the notations above, the following statements are true for an algebraic dynamical system* $(\mathfrak{A}, \alpha_t)$ *with* $\mathfrak{A}$ *a commutative* C^**-algebra*:

(i) *There is an affine bijection between probability measures* μ *on* X *and states on* $\mathfrak{A}$ *given by* $\mu \mapsto \omega_\mu$, *where* $\omega_\mu(A) := \int_X d\mu\, \alpha(A)$.
(ii) *The state* ω_μ *is pure if and only if* μ *is supported at a single point.*
(iii) ω_μ *is an equilibrium state if and only if* $\Psi_t^*\mu = \mu$, *for all* $t \in \mathbb{R}$.
(iv) ω_μ *is a pure equilibrium state if and only if* μ *is supported at a single point in* X_0.
(v) ω_μ *is a ground state if and only if* μ *is supported on* X_0.
(vi) ω *is an extremal ground state if and only if it is pure.*

Proof. We only prove statement (v), as the others follow from standard results on commutative C^*-algebras and the definitions above.[15] By Lemma 2.1, ω_μ is a ground state if and only if $\int_X d\mu\, F(\Psi_t^* G - G) = 0$, for all F, $G \in C(X)$. Because $\Psi_t^* G - G = 0$ on X_0 this is certainly the case when $\mathrm{supp}(\mu) \subset X_0$ (cf. Ref. 15, Remark 3.4.13). Conversely, for any $x \in X_0^c$ in the complement of X_0 we can find a $t \in \mathbb{R}$ and an open set $U \subset X$ such that $x \in U$ and $\Psi_t(U) \cap U = \emptyset$. (In detail: we may first choose a $t \in \mathbb{R}$ such that $y := \Psi_t(x) \neq x$. As X is Hausdorff we may find an open set $V \subset X$ such that $x \in V$ and $y \notin \bar{V}$. Taking $U := V \setminus \Psi_{-t}(\bar{V})$ will do.) By Urysohn's Lemma[24] there is a $G \in C(X)$ with $G(x) = 1$

which vanishes on $X \setminus U$. Note that $\bar{G}\Psi_t^* G = 0$, so if ω_μ is a ground state we have $\int_X d\mu |G|^2 = -\int_X d\mu\, \bar{G}(\Psi_t^* G - G) = 0$. As $G(x) = 1$ this entails that $x \notin \mathrm{supp}(\mu)$, so $\mathrm{supp}(\mu) \subset X_0$. □

Note in particular that pure equilibrium states are automatically ground states.

2.1.2. *KMS states*

In physical applications, thermal equilibrium states can be characterized by the KMS-condition:

Definition 2.4. A state ω on an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$ is called a *β-KMS state* for $\beta > 0$, when it satisfies the *KMS-condition* at *inverse temperature* β, i.e. when for all operators A, $B \in \mathfrak{A}$ there is a holomorphic function F_{AB} on the strip $\mathrm{S}_\beta := \mathbb{R} \times i(0, \beta) \subset \mathbb{C}$ with a bounded, continuous extension to $\overline{\mathrm{S}_\beta}$ such that

$$F_{AB}(t) = \omega(A\alpha_t(B)) , \quad F_{AB}(t + i\beta) = \omega(\alpha_t(B)A) . \tag{2.1}$$

We will denote the space of all β-KMS states by $\mathscr{G}^{(\beta)}(\mathfrak{A})$. A β-KMS state ω is called *extremal* if for any decomposition $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ with $\omega_1, \omega_2 \in \mathscr{G}^{(\beta)}(\mathfrak{A})$ and $0 < \lambda < 1$ we must have $\omega_1 = \omega_2 = \omega$.

When $\mathfrak{A}$ is a topological *-algebra and ω is a continuous state, then it suffices to require the existence of F_{AB} for A, B in a dense subalgebra of $\mathfrak{A}$, as we will see in Proposition 2.1. When $(\mathfrak{A}, \alpha_t)$ is a C^*-dynamical system one may also drop the requirement that F_{AB} is bounded (Ref. 14, Proposition 5.3.7).

The motivations behind this condition will be discussed in some detail in Sec. 6, in the context of our physical applications to the linear scalar quantum field. Note, however, that a ground state satisfies a similar condition with $\beta = \infty$, when we identify S_β, respectively $\overline{\mathrm{S}_\beta}$, with the open, respectively closed, upper half plane. (This may be seen by the same methods as used in the proof of Lemma 2.1.)

The following general result again relies on analytic continuation arguments:

Proposition 2.1. *Let ω be a β-KMS state on an algebraic dynamical system $(\mathfrak{A}, \alpha_t)$. Then the following hold true*:

(i) *ω is an equilibrium state.*
(ii) *For all $A, B \in \mathfrak{A}$ and $z \in \overline{\mathrm{S}_\beta}$ we have*

$$|F_{AB}(z)|^2 \leq \max(\omega(AA^*)\omega(B^*B), \omega(A^*A)\omega(BB^*)) .$$

Proof. For any B the function $F_{IB}(z)$ satisfies $F_{IB}(t) = F_{IB}(t + i\beta)$. Let $F(z)$ be the periodic extension of $F_{IB}(z)$ in $\mathrm{Im}(z)$ with period β. Then F is continuous and bounded on $\mathbb{C}$ and it is holomorphic, even when $\mathrm{Im}(z) \in \beta\mathbb{Z}$, by the Edge of the Wedge Theorem.[23] F must then be a constant by Liouville's Theorem,[23] so $F_{IB}(t) = F_{IB}(0)$, i.e. $\omega(\alpha_t(B)) = \omega(B)$ and ω is in equilibrium.

For any operators $A, B \in \mathfrak{A}$ the corresponding function F_{AB} on $\overline{\mathrm{S}_\beta}$ satisfies

$$|F_{AB}(z)| \leq \sup_{t \in \mathbb{R}} \max\{|F_{AB}(t)|, |F_{AB}(t+i\beta)|\}$$

by the boundedness of F_{AB} and Hadamard's Three Line Theorem (Ref. 21, Appendix to IX.4). The second statement then follows from the first and the Cauchy–Schwarz inequality. $\square$

For commutative algebras a state ω is a β-KMS state if and only if it is a ground state (cf. Lemma 2.1).

2.2. *Weyl C^*-algebras*

For our physical applications to linear scalar quantum fields we will make use of an algebraic formulation involving Weyl C^*-algebras. In preparation for those applications we will now briefly review some fundamental aspects of these algebras,[19] especially in relation to thermal equilibrium states.

We consider a pre-symplectic space (L, σ), which means that L is a real linear space and σ is an antisymmetric bilinear form. We call (L, σ) a symplectic space if σ is nondegenerate, which means that $\sigma(f, f') = 0$ for all $f' \in L$ implies $f = 0$. For each pre-symplectic space (L, σ) there is a unique C^*-algebra generated by linearly independent operators $W(f)$, $f \in L$, subject to the Weyl relations[19]

$$W(f)W(f') = e^{\frac{-i}{2}\sigma(f,f')}W(f+f')\,, \quad W(f)^* = W(-f)\,. \tag{2.2}$$

This is the Weyl C^*-algebra, which we will denote by $\mathcal{W}(L, \sigma)$. By construction, the linear space generated by all $W(f)$, but without taking the completion in the C^*-norm, is also *-algebra, which we will denote by $\mathring{\mathcal{W}}(L, \sigma)$ and which is a dense subset of $\mathcal{W}(L, \sigma)$. Every state on $\mathcal{W}(L, \sigma)$ restricts to a state on $\mathring{\mathcal{W}}(L, \sigma)$, but we even have the following stronger result:

Lemma 2.2. *The restriction map $r : \mathscr{S}(\mathcal{W}(L, \sigma)) \to \mathscr{S}(\mathring{\mathcal{W}}(L, \sigma))$ is an affine homeomorphism for the respective weak*-topologies.*

This follows from Theorem 3.5 and Lemma 3.3(a) of Ref. 19 and the fact that the weak*-topology on a bounded set in the continuous dual space $\mathcal{W}(L, \sigma)'$ is already determined by the dense set $\mathring{\mathcal{W}}(L, \sigma) \subset \mathcal{W}(L, \sigma)$.

The Weyl C^*-algebra $\mathcal{W}(L, 0)$ is commutative, so there is a *-isomorphism $\alpha : \mathcal{W}(L, 0) \to C(X)$, where we may identify X as the space of pure states $\mathscr{S}(\mathcal{W}(L, 0))$. Alternatively we may identify X with the dual group $\hat{L}$ of L, viewed as an additive group.[19] Elements of $\hat{L}$ are characters of L, i.e. group homomorphisms from L (as an additive group) to the unit circle S^1 (as a multiplicative group). The bijection between pure states $\rho \in X$ and characters $\chi \in \hat{L}$ is given by $\rho(W(f)) = \chi(f)$ (cf. Ref. 15, Proposition 4.4.1).

Remark 2.1. For any pure state $\rho \in \mathscr{S}(\mathcal{W}(L,0))$ we can define a *-isomorphism $\eta_\rho : \mathcal{W}(L,\sigma) \to \mathcal{W}(L,\sigma)$ by continuous linear extension of $\eta_\rho(W(f)) := \rho(W(f))W(f)$.[19] The *-isomorphisms η_ρ are sometimes known as *gauge transformations of the second kind*. We will denote the gauge transformations on the commutative Weyl algebra $\mathcal{W}(L,0)$ by ζ_ρ.

The state space $\mathscr{S}(\mathcal{W}(L,0))$ contains a special state,[b] ρ^0, defined by $\rho^0(W(f)) = 1$, for all $f \in L$. This state is pure, because its GNS-representation is one-dimensional. It is easy to verify that $\rho = \zeta_\rho^* \rho^0$ for all pure states $\rho \in \mathscr{S}(\mathcal{W}(L,0))$.

The algebras $\mathcal{W}(L,\lambda\sigma)$, $0 \leq \lambda \leq 1$, may be viewed as a strict and continuous deformation[25] of the commutative algebra $\mathcal{W}(L,0)$. It will be interesting for us to compare the state space of the Weyl C^*-algebra $\mathcal{W}(L,\sigma)$ with that of the commutative Weyl C^*-algebra $\mathcal{W}(L,0)$:

Lemma 2.3. *For every $\omega' \in \mathscr{S}(\mathcal{W}(L,\sigma))$ there is a unique weak*-continuous, affine map $\lambda_{\omega'} : \mathscr{S}(\mathcal{W}(L,0)) \to \mathscr{S}(\mathcal{W}(L,\sigma))$ which is given by $\lambda_{\omega'}(\rho) = \eta_\rho^*\omega'$ on pure states. For any pure state ρ' on $\mathcal{W}(L,0)$ we have $\lambda_{\omega'} \circ \zeta_{\rho'}^* = \eta_{\rho'}^* \circ \lambda_{\omega'}$ and $\lambda_{\omega'}$ is injective when $\omega'(W(f)) \neq 0$, for all $f \in L$.*

Proof. For pure states we have

$$\lambda_{\omega'}(\rho)(W(f)) = \omega'(W(f))\rho(W(f))\,.$$

Because every state in $\mathscr{S}(\mathcal{W}(L,0))$ is a weak*-limit of finite affine combinations of pure states, $\lambda_{\omega'}$ extends uniquely to a weak*-continuous, affine map from $\mathscr{S}(\mathcal{W}(L,0))$ to $\mathscr{S}(\mathcal{W}(L,\sigma))$, which is given by the same formula. The injectivity of $\lambda_{\omega'}$ under the stated assumptions is immediate from this formula and Lemma 2.2. The intertwining relation with the gauge transformations of the second kind is a straightforward exercise. □

2.2.1. *Quasi-free and C^k states*

On any Weyl C^*-algebra there is a special class of states, called quasi-free states, which are distinguished by their algebraic form. They are obtained from the following well known result:

Theorem 2.3. *Let (L,σ) be a pre-symplectic space. A sesquilinear form ω_2 on the complexification $L \otimes \mathbb{C}$ defines a state ω on $\mathcal{W}(L,\sigma)$ by continuous linear extension of*

$$\omega(W(f)) = e^{-\frac{1}{2}\omega_2(f,f)}\,, \quad f \in L\,,$$

[b]Not to be confused with the tracial state ρ^t, defined by $\rho^t(W(f)) = 0$, for all $f \neq 0$, which can be defined on any Weyl C^*-algebra, commutative or not.

if and only if for all $f,\ f' \in L \otimes \mathbb{C}$:

(i) $\omega_2(\bar{f}, f) \geq 0$ (*positive type*),
(ii) $2\omega_{2-}(f, f') := \omega_2(f, f') - \omega_2(f', f) = i\sigma(f, f')$ (*canonical commutator*).

We will call ω_2 a two-point function, even though it is generally not a function of two points $x, y \in M$. The two-point function ω_2 can be characterized alternatively in terms of a one-particle structure:[7]

Definition 2.5. A *one-particle structure* on a pre-symplectic space (L, σ) is a pair $(p, \mathcal{K})$ consisting of a complex linear map $p : L \otimes \mathbb{C} \to \mathcal{K}$ into a Hilbert space $\mathcal{K}$ such that

(i) p has dense range in $\mathcal{K}$,
(ii) $\langle p(\bar{f}), p(f')\rangle - \langle p(\bar{f}'), p(f)\rangle = i\sigma(f, f')$.

Given a one-particle structure, one can define an associated two-point function by setting $\omega_2(\bar{f}, f') := \langle p(f), p(f')\rangle$. Conversely, a two-point function ω_2 determines a unique one-particle structure $(p, \mathcal{K})$ such that the above equality holds, by similar arguments as used in the GNS-construction. We call this as the one-particle structure associated with ω_2.

A wider class of states which will be of interest is the following:

Definition 2.6. A state ω on the Weyl C^*-algebra $\mathcal{W}(L, \sigma)$ is called C^k, $k > 0$, when the maps

$$\omega_n(f_1, \ldots, f_n) := (-i)^n \partial_{s_1} \cdots \partial_{s_n} \omega(W(s_1 f_1) \cdots W(s_n f_n))|_{s_1 = \cdots = s_n = 0}$$

are well defined on $C_0^\infty M^{\times n}$ for all $1 \leq n \leq k$. The ω_n are linear maps and they are called the n-point functions. A state is called C^∞, when it is C^k for all $k > 0$.

When ω is a quasi-free state, it is C^∞ and all higher n-point functions can be expressed in terms of the two-point function ω_2 via Wick's Theorem. For such states it only remains to analyze the two-point functions ω_2.

A physical reason why quasi-free states are of interest is the following (see also Theorems 5.1 and 6.2):

Theorem 2.4. *Let* (L, σ) *be a pre-symplectic space and let* ω *be a* C^2 *state on* $\mathcal{W}(L, \sigma)$. ω_2, *as defined in Definition* 2.6, *defines a unique quasi-free state* ω' *by Theorem* 2.3 *and a one-particle structure* $(p, \mathcal{K})$. *Then,*

(i) ω' *is pure if and only if* p *has a dense range already on* L (*without complexification*) *and* $p(f) = 0$ *for all degenerate* $f \in L$ (*i.e.* $f \in L$ *for which* $\sigma(f, f') = 0$ *for all* $f' \in L$).
(ii) *If* ω' *is pure, then* $\omega = \omega'$.

Proof. The claim that ω_2 satisfies the assumptions of Theorem 2.3 is a standard exercise. The characterization of pure quasi-free states in terms of their one-particle structures was established in Ref. 8, Lemma A.2, for the symplectic case. The generalization to the pre-symplectic case is straightforward. The fact that this implies that $\omega = \omega'$ is a theorem due to Ref. 26, for the symplectic case. This result and its proof carry over to the pre-symplectic case without modification. $\square$

A related result in the commutative case is the following characterization of the state ρ^0:

Proposition 2.2. *If $\rho \in \mathscr{S}(\mathcal{W}(L,0))$ is a C^1 pure state, then $\rho(W(f)) = e^{i\rho_1(f)}$ for all $f \in L$. In particular, if $\rho_1 = 0$, then $\rho = \rho^0$.*

Proof. Given any $f \in L$ we consider $F(t) := \rho(W(tf))$. Because ρ is pure and $\mathcal{W}(L,0)$ is commutative, $F(t+t') = F(t)F(t')$ (cf. Ref. 15, Proposition 4.4.1) and since ρ is C^1, F is continuous at $t=0$ and hence everywhere. Furthermore, $\partial_t F(t) = F(t)\partial_t F(0) = F(t) i\rho_1(f)$ and therefore $F(t) = e^{it\rho_1(f)}$, so the results follow. $\square$

2.3. *Quasi-free dynamics on Weyl C^*-algebras*

A pre-symplectic isomorphism T of (L,σ) is a real-linear isomorphism $T : L \to L$ which preserves the pre-symplectic form, $\sigma(Tf, Tf') = \sigma(f, f')$. Each pre-symplectic isomorphism gives rise to a unique *-isomorphism α_T of $\mathcal{W}(L,\sigma)$ such that $\alpha_T(W(f)) = W(Tf)$ (see Ref. 19 or also Ref. 14, Theorem 5.2.8). Hence, a one-parameter group of pre-symplectic isomorphisms T_t gives rise to a one-parameter group α_t of *-isomorphisms on $\mathcal{W}(L,\sigma)$. Not every one-parameter group of *-isomorphisms on $\mathcal{W}(L,\sigma)$ arises in this way, but the time evolution that we will be interested in for our physical applications does.

Definition 2.7. A *one-particle dynamical system* (L,σ,T_t) is a one-parameter group of pre-symplectic isomorphisms T_t on a pre-symplectic space (L,σ). The associated algebraic dynamical system $(\mathcal{W}(L,\sigma),\alpha_t)$ with $\alpha_t(W(f)) = W(Tf)$ is called *quasi-free*.

An equilibrium one-particle structure $(p,\mathcal{K})$ on a one-particle dynamical system (L,σ,T_t) is a one-particle structure on (L,σ) for which there is a one-parameter unitary group $\tilde{O}_t$ on $\mathcal{K}$ such that $\tilde{O}_t p = pT_t$.

A *ground one-particle structure* is an equilibrium one-particle structure $(p,\mathcal{K})$ for which the unitary group $\tilde{O}_t = e^{itH}$ is strongly continuous and $H \geq 0$.

A *KMS one-particle structure* at inverse temperature $\beta > 0$ is an equilibrium one-particle structure $(p,\mathcal{K})$, with associated two-point function ω_2, such that for all $f, f' \in L$ there exists a bounded continuous function $F_{ff'}$ on $\overline{\mathrm{S}_\beta}$, holomorphic on its interior, satisfying

$$F_{ff'}(t) = \omega_2(f, T_t f')\,, \quad F_{ff'}(t+i\beta) = \omega_2(T_t f', f)\,.$$

An equilibrium one-particle structure is called *nondegenerate* when $\tilde{O}_t = e^{itH}$ is strongly continuous and 0 is not an eigenvalue for H.

Note that a quasi-free state ω with two-point function ω_2 is in equilibrium for a quasi-free dynamical system if and only if the associated one-particle structure $(p, \mathcal{K})$ is in equilibrium. Furthermore, we have

Proposition 2.3. *Let ω be a C^2 equilibrium state on a quasi-free algebraic dynamical system $(\mathcal{W}(L, \sigma), \alpha_t)$. Let $(p, \mathcal{K})$ be the one-particle structure associated to ω_2 and assume that $\omega_1 = 0$.*

(i) *If ω is a (nondegenerate) ground state, then $(p, \mathcal{K})$ is a (nondegenerate) ground one-particle structure.*
(ii) *If ω is a β-KMS state, then $(p, \mathcal{K})$ is a β-KMS one-particle structure.*

When ω is quasi-free, the converses of these statements are also true.

Proof. We may identify $\mathcal{K}$ as a closed linear subspace of the GNS-representation space $\mathcal{H}_\omega$, spanned by the vectors $p(f) := \Phi_\omega(f)\Omega_\omega := -i\partial_s \pi_\omega(W(sf))\Omega_\omega|_{s=0}$. This derivative is well defined, because ω is C^2. The unitary group U_t on $\mathcal{H}_\omega$ restricts to a unitary group $\tilde{O}_t$ on $\mathcal{K}$, because the dynamics is quasi-free, and the generator h of U_t restricts to the generator H of $\tilde{O}_t$. Also note that $\mathcal{K}$ is perpendicular to Ω_ω, because $\omega_1 = 0$. It is then clear that when ω is a (nondegenerate) ground state, then H is (strictly) positive and $(p, \mathcal{K})$ is a (nondegenerate) ground one-particle structure. When ω is a β-KMS state and f, $f' \in L$, we may take $A(s) := s^{-1}(W(sf) - I)$ and $B(s) := s^{-1}(W(sf') - I)$ for any $s \neq 0$ to find functions $F_{A(s)B(s)}$. Because ω is C^2, the functions $\omega(A^*(s)A(s))$ and $\omega(A(s)A^*(s))$ have well defined limits as $s \to 0$, and similarly for B. We may then use Proposition 2.1 to take the uniform limit of $-F_{A(s)B(s')}$ as $s, s' \to 0$, which yields the desired function $F_{ff'}$. This proves both items.

If ω is quasi-free, its GNS-representation is a Fock space, $\mathcal{H}_\omega = \oplus_{n=0}^{\infty} P_{+,n}\mathcal{K}^{\otimes n}$, where $P_{+,n}$ is the projection onto the symmetrized n-fold tensor product. U_t is the second quantization of $\tilde{O}_t$ and h is the second quantization of H. For the converse of the first statement we note that ω is a (nondegenerate) ground state if and only if the restriction of h to each n-particle space with $n \geq 1$ is (strictly) positive. If $(p, \mathcal{K})$ is a (nondegenerate) ground one-particle structure, then H is (strictly) positive. The restriction h_n of h to $P_{+,n}\mathcal{K}^{\otimes n}$ is given by $\overline{H_n} P_{+,n}$, where H_n is defined to be the operator $H_n := \sum_{j=1}^{n} I^{\otimes j-1} \otimes H \otimes I^{\otimes n-j}$ on the algebraic tensor product $D(H)^{\otimes n}$ of the domain $D(H)$ of H. By Nelson's Analytic Vector Theorem (Ref. 21, Theorem X.39), H_n is essentially self-adjoint (because H is). The closure of each summand in H_n is a (strictly) positive operator (by Lemma A.3), and hence so is $\overline{H_n}$ (by Lemma A.6). Therefore, h_n is (strictly) positive for $n \geq 1$ and ω is a (nondegenerate) ground state.

Now we turn to the converse of the second statement. One may use the Weyl relations and the quasi-free property to find

$$\omega(W(f)\alpha_t(W(f'))) = \omega(W(f))\omega(W(f'))e^{-\omega_2(f, T_t f')}.$$

Using $F_{ff'}$ in the exponent yields the desired $F_{W(f)W(f')}$. For finite linear combinations of Weyl operators the desired property is now clear and for general operators in $\mathcal{W}(L,\sigma)$ one appeals to Proposition 2.1 and a limiting argument. □

One of the nice aspects of quasi-free dynamical systems is that we may view T_t also as a pre-symplectic isomorphism of $(L,0)$, so we may compare the corresponding quasi-free dynamics on $\mathcal{W}(L,\sigma)$ and on $\mathcal{W}(L,0)$. In this context we prove the following result (adapted from Ref. 27):

Proposition 2.4. *Let (L,σ,T_t) be a one-particle dynamical system and consider the corresponding quasi-free dynamical systems $(\mathcal{W}(L,\sigma),\alpha_t)$ and $(\mathcal{W}(L,0),\beta_t)$.*

(i) *If $\omega^{(\beta)}\in\mathscr{G}^{(\beta)}(\mathcal{W}(L,\sigma))$ is quasi-free and $\omega_2^{(\beta)}$ defines a nondegenerate equilibrium one-particle structure, then the map $\lambda_{(\beta)}:=\lambda_{\omega^{(\beta)}}$ of Lemma 2.3 restricts to an affine homeomorphism $\lambda_{(\beta)}:\mathscr{G}^0(\mathcal{W}(L,0))\to\mathscr{G}^{(\beta)}(\mathcal{W}(L,\sigma))$.*
(ii) *If $\omega^0\in\mathscr{G}^0(\mathcal{W}(L,\sigma))$ is quasi-free and nondegenerate and the strong derivative $\partial_t\pi_{\omega^0}(\alpha_t(W(f)))\Omega_{\omega^0}|_{t=0}$ exists for all $f\in L$, then the map $\lambda_0:=\lambda_{\omega^0}$ restricts to an affine homeomorphism $\lambda_0:\mathscr{G}^0(\mathcal{W}(L,0))\to\mathscr{G}^0(\mathcal{W}(L,\sigma))$.*

Proof. First consider the KMS case. It follows from Lemma 2.3 that $\lambda_{(\beta)}$ defines a continuous affine map from $\mathscr{G}^0(\mathcal{W}(L,0))$ to $\mathscr{S}(\mathcal{W}(L,\sigma))$, which is injective because $\omega^{(\beta)}(W(f))=e^{-\frac{1}{2}\omega_2^{(\beta)}(f,f)}\neq 0$. If $\rho\in\mathscr{G}^0(\mathcal{W}(L,0))$, then $\omega:=\lambda_{(\beta)}(\rho)$ is invariant under α_t, because $\omega^{(\beta)}$ and ρ are equilibrium states for α_t and β_t, respectively, and these one-parameter groups are quasi-free with the same underlying T_t. For any $A=\sum_{i=1}^n c_iW(f_i)$ and $B=\sum_{i=1}^n d_iW(f_i')$ in $\mathring{\mathcal{W}}(L,\sigma)$ we have

$$\omega(A\alpha_t(B))=\sum_{i,j=1}^n c_id_j\omega^{(\beta)}\big(W(f_i)\alpha_t\big(W(f_j')\big)\big)\rho\big(W(f_i)W(f_j')\big)\,, \tag{2.3}$$

by a short computation involving the Weyl relations and the properties of ρ established in Lemma 2.1. A similar computation for $\omega(\alpha_t(B)A)$ and the KMS-condition for $\omega^{(\beta)}$ now imply the existence of a function F_{AB} as needed for the KMS-condition for ω. For the operators in the C^*-algebraic completion $\mathcal{W}(L,\sigma)$ one uses Proposition 2.1. Hence ω is a β-KMS state.

For ground states, Eq. (2.3) (with ω^0 instead of $\omega^{(\beta)}$) implies that the unitary group U_t that implements α_t in the GNS-representation of ω is weakly continuous and hence strongly continuous. The dense domain $\pi_\omega(\mathcal{W}(L,\sigma))\Omega_\omega$ is invariant under the action of U_t and one may show that $U_t=e^{ith}$ has strong derivatives there, because the same is true for ω^0. Hence this domain is a core for the Hamiltonian h (see e.g. Theorem VIII.10 of Ref. 21). Taking the derivative with respect to t of Eq. (2.3) and taking $A=B$ shows that $h\geq 0$, by Schur's Product Theorem (cf. Ref. 28, Chap. 6, Sec. 7 or Ref. 29). This proves that ω is a ground state.

We now turn to surjectivity. Given any $\omega\in\mathscr{G}^{(\beta)}(\mathcal{W}(L,\sigma))$ we may define the linear map ρ on $\mathring{\mathcal{W}}(L,0)$ by $\rho(W(f)):=\frac{\omega(W(f))}{\omega^{(\beta)}(W(f))}$ for all $f\in L$. Given any $f,\,f'\in L$

we now let $F^{(\beta)}_{W(-f)W(f')}(z)$ and $F_{W(-f)W(f')}(z)$ be the functions on $\overline{\mathrm{S}_\beta}$, obtained from the KMS-condition for $\omega^{(\beta)}$ and ω, respectively. Note that $F^{(\beta)}_{W(-f)W(f')}(z) = C\exp(-F_{-f,f'}(z))$, by the one-particle KMS-condition for ω_2 (cf. Proposition 2.3), where $C := \exp\left(-\frac{1}{2}(\omega^{(\beta)}(f,f) + \omega^{(\beta)}(f',f'))\right)$. Hence,

$$G(z) := \left(F^{(\beta)}_{W(-f)W(f')}(z)\right)^{-1} F_{W(-f)W(f')}(z)$$

defines a bounded and continuous function on $\overline{\mathrm{S}_\beta}$ which is holomorphic in its interior. Furthermore, $G(t) = \rho(W(-f)\beta_t(W(f')))$ and $G(t+i\beta) = \rho(\beta_t(W(f'))W(-f))$. As ρ is defined on a commutative C^*-algebra it then follows that $G(z+i\beta) = G(z)$ and we may extend G periodically to a bounded continuous function on $\mathbb{C}$, which is entire holomorphic by the Edge of the Wedge Theorem.[23] Hence, G is constant (by Liouville's Theorem[23]) and $\rho(W(-f)\beta_t(W(f')) = \rho(W(-f)W(f'))$ for all $t \in \mathbb{R}$. A similar argument holds for the case of ground states.

For any $A = \sum_{i=1}^n c_i W(f_i)$ we have

$$\begin{aligned} 0 &\leq \sum_{i,j=1}^N \overline{c_i} c_j \omega(W(-f_i)W(f_j)) \\ &= \sum_{i,j=1}^N \overline{c_i} c_j \exp\left(-\frac{1}{2}\omega_2^{(\beta)}(f_j - f_i, f_j - f_i)\right)\rho(W(-f_i)W(f_j)) . \end{aligned}$$

For some $t > 0$, we now let $F_i^M := \sum_{m=0}^{M-1} \frac{1}{M} T_{mt} f_i$ for any $M \in \mathbb{N}$. Using the previous paragraph one shows that $\rho\big(W\big(-F_i^M\big)W\big(F_j^M\big)\big) = \rho(W(-f_i)W(f_j))$, from which we find

$$0 \leq \sum_{i,j=1}^N \overline{c_i} c_j \exp\left(-\frac{1}{2}\omega_2^{(\beta)}\left(F_j^M - F_i^M, F_j^M - F_i^M\right)\right)\rho(W(-f_i)W(f_j)) .$$

However, as the one-particle structure $(p, \mathcal{K})$ associated to $\omega_2^{(\beta)}$ is nondegenerate, we see from von Neumann's Mean Ergodic Theorem (Ref. 21, Theorem II.11) that $\lim_{M\to\infty} p(F_i^M) = 0$. The exponential term will then converge to 1 as $M \to \infty$, leading to the conclusion that ρ is positive. The unique extension of ρ to a state on $\mathcal{W}(L,0)$ is a ground state by the result of the previous paragraph and Lemma 2.1. The same argument works for the case of ground states.

Finally, to see that $\lambda_{(\beta)}$ (respectively λ_0) is a homeomorphism it suffices to note that the inverse map $\omega \mapsto \rho$ is weak *-continuous from $\mathscr{G}^{(\beta)}(\mathring{\mathcal{W}}(L,\sigma))$ (respectively $\mathscr{G}^0(\mathring{\mathcal{W}}(L,\sigma))$) to $\mathscr{G}^0(\mathring{\mathcal{W}}(L,0))$, by construction. $\square$

Remark 2.2. In the setting of Proposition 2.4 we note that the space $\mathscr{G}^0(\mathcal{W}(L,0))$ of classical ground states always contains the pure state ρ^0 and that $\omega^{(\beta)} = \lambda_{(\beta)}(\rho^0)$. For any other pure classical ground state $\rho \in \mathscr{G}^0(\mathcal{W}(L,0))$ we consider the gauge transformations of the second kind η_ρ of $\mathcal{W}(L,\sigma)$ and ζ_ρ of $\mathcal{W}(L,0)$ (cf. Remark 2.1).

We then have $\rho = \zeta_\rho^* \rho^0$ and $\lambda^{(\beta)} \circ \zeta_\rho^* = \eta_\rho^* \circ \lambda^{(\beta)}$. Thus every extremal β-KMS state can be obtained from $\omega^{(\beta)}$ by a gauge transformation of the second kind. The same holds for extremal ground states and ω^0. In particular, all extremal ground states are pure.

3. Review of Geometric Results

Before we consider the details of the linear scalar quantum field it is in order to study the space–time in which it propagates. In the paragraphs below we will describe the class of stationary, globally hyperbolic space–times and the subclass of standard static space–times. For the latter case we also introduce the complexification and Euclideanization that are necessary in order to perform a Wick rotation. Most of our exposition here is a brief review of recent results of Refs. 30 and 31.

We assume that the reader is already familiar with the following standard terminology, which will be used throughout (cf. Ref. 32):

Definition 3.1. A *space–time* $M = (\mathcal{M}, g)$ is a smooth, connected, oriented manifold $\mathcal{M}$ of dimension $d \geq 2$ with a smooth Lorentzian metric g of signature $(- + \cdots +)$.

A *Cauchy surface* Σ in M is a subset $\Sigma \subset M$ that is intersected exactly once by every inextendible time-like curve in M. A space–time is said to be *globally hyperbolic* when it has a Cauchy surface.

For a space–time M we note that the manifold $\mathcal{M}$ is automatically paracompact.[33] We are mainly interested in space–times that are globally hyperbolic, because they allow us to formulate the linear field equation as an initial value (or Cauchy) problem. We will only consider Cauchy surfaces that are space-like, smooth hypersurfaces.[34] A globally hyperbolic space–time is automatically time-orientable and we will assume that a choice of time-orientation has been fixed. It follows that any Cauchy surface is also oriented. Our notions and notations for causal relations, the Levi-Civita connection, etc. follow standard usage.[32] We will let h denote the Riemannian metric on a Cauchy surface Σ induced by the Lorentzian metric g on M, and we let $\nabla^{(h)}$ denote the corresponding Levi-Civita connection on Σ. Space–time indices $a, b, \ldots$ are chosen from the beginning of the alphabet and run from 0 to $d-1$, whereas spatial indices are denoted by $i, j, \ldots$ and run from 1 to $d-1$.

3.1. *Stationary space–times*

Stationary space–times come equipped with a preferred notion of time-flow, which is mathematically encoded in the presence of a time-like vector field. To be precise:

Definition 3.2. A *stationary space–time* (M, ξ) is a space–time M together with a smooth, complete, future-pointing, time-like Killing vector field ξ on M.

Here completeness means that the corresponding flow $\Xi : \mathbb{R} \times \mathcal{M} \to \mathcal{M}$, defined by $\Xi(0, x) = x$ and $d\Xi(t, x; \partial_t, 0) = \xi(\Xi(t, x))$, is well defined for all $t \in \mathbb{R}$. This flow is interpreted physically as the flow of time and following standard usage we write $\Xi_t : \mathcal{M} \to \mathcal{M}$ for the map $\Xi_t(x) := \Xi(t, x)$.

ξ is a Killing vector field if it satisfies Killing's equation, $\nabla_{(a}\xi_{b)} = 0$, where the round brackets in the subscript denote symmetrization as an idempotent operation. Equivalently, it means that the metric is invariant under the time flow of ξ, $\Xi_t^* g = g$ for all $t \in \mathbb{R}$.

Example 3.1 (Standard stationary space–times). Examples of stationary space–times are easily obtained by the following construction. Let S be a manifold of dimension $d-1$, let h be a Riemannian metric on S, let $v > 0$ be a smooth, strictly positive function on S and let w be a smooth one-form on S such that $h^{ij}w_i w_j < v^2$. One now defines $\mathcal{M} := \mathbb{R} \times S$ with canonical projection map $\pi : \mathcal{M} \to S$ and the canonical time coordinate $t : \mathcal{M} \to \mathbb{R}$ is the canonical projection onto the first factor. A stationary space–time $M = (\mathcal{M}, g)$ is then obtained by defining

$$g := -(\pi^* v)^2 dt^{\otimes 2} + 2\pi^*(w) \otimes_s dt + \pi^* h \,,$$

where $\otimes_s$ is the symmetrized tensor product. We will always choose adapted local coordinates on M, i.e. coordinates (t, x^i) such that the x^i are local coordinates on S, unless stated otherwise.

Note that g indeed has a Lorentz signature and that the canonical vector field ∂_t on $\mathbb{R}$ gives rise to a Killing vector field ξ on M. On $S_0 := \{0\} \times S$ we can write $\xi^a = Nn^a + N^a$, where n^a is the future pointing unit normal vector field to $S_0 \subset M$ and $n_a N^a = 0$. The function N is known as the lapse function and N^a as the shift vector field. They are related to v and w by

$$N = (v^2 + h^{ij} w_i w_j)^{\frac{1}{2}} \,, \quad N^i = h^{ij} w_j \,,$$

where we use the fact that N^a is tangent to Σ, so the component for $a = 0$ vanishes (in adapted local coordinates). The inverse of the metric takes the form

$$g^{-1} = -N^{-2} \partial_t^{\otimes 2} + 2N^{-2} N^j \partial_j \otimes_s \partial_t + (h^{ij} - N^{-2} N^i N^j) \partial_i \otimes \partial_j \,,$$

where h^{ij} is the inverse of the Riemannian metric h.

Definition 3.3. A stationary space–time of the form of Example 3.1 is called a *standard stationary space–time.*

Note that a standard stationary space–time M is uniquely determined by the data (S, h, v, w). However, different data may give rise to the same space–time, because there is a lot of freedom in the choice of the surface $S \subset M$. This is another way of saying that a stationary space–time has a preferred time-flow, given by the Killing vector field, but it does not have a preferred time coordinate, because we can choose different canonical time coordinates which vanish on different spatial hypersurfaces.

Although not all stationary space–times are standard,[c] they are the only ones of interest to us because of the following result:

Proposition 3.1. *Let M be a stationary space–time which is globally hyperbolic. Then M is isometrically diffeomorphic to a standard stationary space–time.*

This is Proposition 3.3 of Ref. 31. The proof is elegant and short and we include it here for completeness:

Proof. Fix a Cauchy surface $\Sigma \subset M$ and use the flow Ξ of the Killing vector field to define a local diffeomorphism $\psi : \mathbb{R} \times \Sigma \to M$ by $\psi(t, x) = \Xi(t, x)$. The curves $t \mapsto \psi(t, x)$ are time-like and inextendible, because ξ is assumed to be complete. This means that they intersect Σ exactly once, proving that ψ is both injective and surjective and hence a diffeomorphism. We define $M' := (\mathbb{R} \times \Sigma, \psi^* g)$ and it remains to show that M' is standard stationary. This follows easily from the fact that $\psi^*\xi = \partial_t$, where t is the canonical time-coordinate on M', together with the fact that $\partial_t \psi^* g = 0$, which is Killing's equation. □

A more complicated issue is the converse question, whether a standard stationary space–time is globally hyperbolic. A full characterization of those data (S, h, v, w) that give rise to a standard stationary space–time M which is globally hyperbolic was recently given by Ref. 30. It should be noted that S need not be a Cauchy surface, even if M is globally hyperbolic. A full characterization of those data for which S is a Cauchy surface was also given in Ref. 30. To close this section we will sketch the main ingredients of this analysis and state the main results, although they will not be needed in the remainder of this paper.

Let $s \mapsto \gamma(s) := (t(s), x(s))$ be a smooth, time-like curve in a standard stationary space–time M with data (S, h, v, w). The fact that γ is time-like can be stated as the quadratic inequality

$$h_{ij}\dot{x}^i\dot{x}^j + 2w_i\dot{x}^i\dot{t} - v^2\dot{t}^2 \leq 0\,,$$

where $\dot{}$ denotes a derivative with respect to s. If γ is future pointing this leads to

$$\dot{t} \geq v^{-2}w_i\dot{x}^i + \left(v^{-4}(w_i\dot{x}^i)^2 + v^{-2}h_{ij}\dot{x}^i\dot{x}^j\right)^{\frac{1}{2}} =: F(\dot{x})\,,$$

whereas for past-pointing γ we find

$$\dot{t} \leq v^{-2}w_i\dot{x}^i - \left(v^{-4}(w_i\dot{x}^i)^2 + v^{-2}h_{ij}\dot{x}^i\dot{x}^j\right)^{\frac{1}{2}} =: -\tilde{F}(\dot{x})\,.$$

F and $\tilde{F}$ are smooth, strictly positive functions on $TS \setminus 0$, where 0 denotes the zero section. (In fact, F and $\tilde{F}$ define Finsler metrics on S of Randers type. We refer the interested reader to Ref. 30 for a brief introduction or to Ref. 35 for a full exposition on Finsler geometry.)

[c]Consider e.g. Minkowski space–time and compactify an inertial time coordinate to a circle.

It turns out that the questions concerning the causality of the standard stationary space–time with data (S, h, w, v) can be determined entirely from the properties of S with respect to F and $\tilde{F}$. As for a Riemannian metric, we can use F to define the length of a smooth curve $\gamma\colon [0,1] \to S$ as $l_F(\gamma) := \int_0^1 F(\dot{\gamma}(s))ds$ and from that we can define a generalized distance function

$$d(p,q) := \inf_{\gamma \in C(p,q)} l_F(\gamma)\,,$$

where $C(p,q)$ is the set of all piecewise smooth curves from p to q. d satisfies all properties of a distance function, except symmetry. Indeed, if $\tilde{\gamma}(s) := \gamma(1-s)$ we have $l_F(\tilde{\gamma}) = l_{\tilde{F}}(\gamma)$, which in general differs from $l_F(\gamma)$. However, taking the ordering into account one can still define notions of forward and backward Cauchy sequences and corresponding notions of forward and backward completeness for the pair (S, F).[30,35]

We now state without proof the results on the causality of standard stationary space–times (Theorem 4.3b, Theorem 4.4 and Corollary 5.6 of Ref. 30).

Theorem 3.1. *Let M be a standard stationary space–time with data (S, h, v, w).*

(i) *M is globally hyperbolic if and only if for all $x \in S$ and all $r > 0$ the symmetrized closed ball $B_s(p,r) := \{x \mid d(p,x) + d(x,p) \leq r\}$ is compact.*
(ii) *$S \subset M$ is a Cauchy surface if and only if (S, F) is both forward and backward complete. In this case all hypersurfaces $S_t := \{t\} \times S$ are Cauchy.*
(iii) *If M is globally hyperbolic, then $(S, \tilde{h})$ is a complete Riemannian manifold with*

$$\tilde{h} := v^{-2}h + v^{-4}w \otimes w\,.$$

We record for completeness that the inverse metric of $\tilde{h}$ is given by $\tilde{h}^{ij} = v^2h^{ij} - v^2N^{-2}N^iN^j = v^2g^{ij}$, where g^{ij} is expressed in adapted coordinates.

3.2. *Standard static space–times*

We have seen that stationary space–times have a preferred time flow, but no preferred time coordinate. This is different for standard static space–times, which we will describe now. For a full discussion of static space–times we refer the reader to Ref. 31 and references therein.

Definition 3.4. A *static space–time* $M = (\mathcal{M}, g, \xi)$ is a stationary space–time with a Killing vector field ξ that is irrotational.

The property that ξ is irrotational means that the distribution of vectors orthogonal to ξ is involutive, i.e. $[X,Y]^a\xi_a = 0$ when $X^a\xi_a = Y^a\xi_a = 0$. This can be expressed equivalently as

$$\xi_{[a}\nabla_b\xi_{c]} = 0\,,$$

where the square brackets in the subscript denote antisymmetrization as an idempotent operation. By Frobenius' Theorem (Ref. 32, Theorem B.3.2) ξ is irrotational if and only if M can be foliated by hypersurfaces orthogonal to ξ.

If x^i, $i = 1, \ldots, d-1$, are local coordinates on a $(d-1)$-dimensional hypersurface $H \subset M$ orthogonal to ξ we can (locally) supplement them by the parameter t appearing in the flow Ξ_t to define coordinates on a portion of M. When used like this, we call t a Killing time coordinate. Note that the surfaces of constant t remain orthogonal to $\xi = \partial_t$, because they are the image of H under Ξ_t.

Remark 3.1. Although the definition of a (local) Killing time coordinate depends on the choice of the hypersurface H, any two Killing time coordinates on the same open set differ at most by a constant, because both are constant on the hypersurfaces orthogonal to ξ. In this sense, static space–times have a preferred time coordinate up to a constant, which we will often call *the* Killing time coordinate, with some slight abuse of language.

In the local coordinates (t, x^i) the metric can be expressed as

$$g = -v^2\, dt^{\otimes 2} + g_{ij}\, dx^i \otimes dx^j\,,$$

with $1 \leq i, j \leq d-1$ and the smooth coefficient functions v, g_{ij} are independent of t. We introduce a special name for the class of static space–times for which this form of the metric can be obtained globally:

Definition 3.5. A *standard static space–time* $M = (\mathcal{M}, g, \xi)$ is a standard stationary space–time with a vanishing shift vector field, i.e. $\mathcal{M} \simeq \mathbb{R} \times S$, $\xi = \partial_t$ and

$$g = -(\pi^* N)^2 dt^{\otimes 2} + \pi^* h\,,$$

where the Killing time coordinate t is the projection on the first factor of $\mathbb{R} \times S$, π is the projection on the second factor, h is a Riemannian metric on S and N is a smooth, strictly positive function on S.

The data (S, h, N) determine a unique standard static space–time, which is the standard stationary space–time with data $(S, h, v = N, w = 0)$. The canonical time coordinate of the latter coincides with the Killing time coordinate.

Unlike the stationary case, there is only a limited freedom in the choice of data that describe a fixed standard static space–time M. Indeed, suppose that (S, h, v) and (S', h', v') determine the same standard static space–time M and consider the hypersurfaces $S_0 = \{0\} \times S$ and $S'_0 = \{0\} \times S'$ in M. By Remark 3.1 there is a $T \in \mathbb{R}$ such that the diffeomorphism Ξ_T of M has $S'_0 = \Xi_T(S_0)$, $\Xi_T^* h' = h$ and $\Xi_T^* v' = v$.

For our applications to Wick rotations we are particularly interested in space–times which are both standard static and globally hyperbolic. To determine whether a standard static space–time is globally hyperbolic we quote from Theorem 3.1 in Ref. 31:

Theorem 3.2. *For a standard static space–time M with data (S, h, v) the following are equivalent*:

(i) *M is globally hyperbolic.*
(ii) *S is complete in the conformal metric $\tilde{h}_{ij} = v^{-2} h_{ij}$.*
(iii) *Each constant Killing time hypersurface is Cauchy.*

This is in fact a special case of Theorem 3.1, when $w = 0$. In the ultra-static case $v \equiv 1$, it essentially reduces to Proposition 5.2 in Ref. 7. Note, however, that (S, h) itself need not be a complete Riemannian manifold in general.

Remark 3.2. The metric $\tilde{h}$ is also called the optical metric,[36] because geodesics of $\tilde{h}$ are the projections onto Σ of light-like geodesics in M. To see this we first note that the light-like geodesics of $M = (\mathcal{M}, g)$ coincide with those of $\tilde{M} := (\mathcal{M}, v^{-2} g)$ after a reparametrization (cf. Ref. 32, App. D). Because $\tilde{M}$ is ultra-static, the geodesic equation for a curve $\gamma(s) = (t(s), x(s))$ decouples into the geodesic equation for x in $(S, \tilde{h})$ and $\partial_s^2 t = 0$. (Reference 36 also uses the term optical metric in the stationary case for the metric $N^{-2} h$, although the motivation is less convincing in that case. It might be more appropriate to refer to the Finsler metrics F, $\tilde{F}$ of Subsec. 3.1 as optical metrics.)

When the space–time M is both globally hyperbolic and static, it is automatically a standard *stationary* space–time by Proposition 3.1. However, it may yet fail to be a standard static space–time. A simple counterexample, taken from Ref. 37 (see also Ref. 31), is the cylinder space–time $M = (\mathbb{R} \times \mathbb{S}^1, g)$ with the metric $g := -dt^{\otimes 2} + d\theta^{\otimes 2} + 2dt \otimes_s d\theta$. This is a globally hyperbolic space–time with Cauchy surfaces diffeomorphic to the circle $\mathbb{S}^1$. The vector field $\xi = \partial_t$ is a time-like Killing field, which is irrotational on dimensional grounds. However, hypersurfaces orthogonal to ξ must be diffeomorphic to $\mathbb{R}$, as they wind around the cylinder.

A complete characterization of which static, globally hyperbolic space–times are standard static is given by

Proposition 3.2. *Let (M, ξ) be a static, globally hyperbolic space–time. Then M is isometrically diffeomorphic to a standard static space–time if and only if it admits a Cauchy surface that is Killing field orthogonal.*

Proof. If M is isometrically diffeomorphic to a standard static space–time, the existence of a Killing field orthogonal Cauchy surface follows from Theorem 3.2. Conversely, if such a Cauchy surface exists we may choose this surface in the proof of Proposition 3.1, which simultaneously shows that M is isometrically diffeomorphic to a standard stationary space–time M' and that the metric g' has no cross terms involving w. Hence, M' is standard static. □

3.3. *Space–time complexification*

To conclude our geometric considerations we now define complexifications and Riemannian manifolds associated to any given standard static space–time. With a view to our applications to thermal states it is necessary to consider the case where the domain of the imaginary time variable is compactified. For this purpose we let $R > 0$ and we define the cylinder

$$\mathcal{C}_R := \mathbb{C}/\sim\,, \quad z \sim z' \Leftrightarrow z - z' \in 2\pi i R\mathbb{Z}\,.$$

This equivalence relation compactifies the imaginary axis of $\mathbb{C}$ to a circle $\mathbb{S}^1_R$ of circumference $2\pi R$. $\mathcal{C}_\infty := \mathbb{C}$ can be taken as a degenerate case with $R = \infty$ and $\mathbb{S}^1_\infty := \mathbb{R}$.

Let M be a standard static space–time with data (S, h, N). For any $R > 0$ we define the complexification M^c_R as the real manifold $M^c_R = \mathcal{C}_R \times S$ endowed with the symmetric, complex-valued, tensor field

$$g^c_R(z, x) = -N^2(x)(dt + id\tau)^{\otimes 2} + h(x)\,,$$

where $z = t + i\tau$ is the coordinate on $\mathcal{C}_R$. M can be embedded into M^c_R as the $\tau = 0$ surface and g^c_R is the analytic continuation of g in z. Furthermore, we define the Riemannian manifold $M_R := \{(z, x) \in M^c_R |\ t = 0\}$ endowed with the pull-back metric of g^c_R

$$g_R(\tau, x) = N^2(x)d\tau^{\otimes 2} + h(x)\,.$$

Note that $M_R \simeq \mathbb{S}^1_R \times S$ as a manifold and since $S = M \cap M_R$ in M^c_R, we can identify S also as the $\{\tau = 0\}$ surface in M_R. M_R has a Killing field $\xi_R = \partial_\tau$, which can be viewed as the analytic continuation of $\xi = \partial_t$.

The constructions above do not depend on any freedom in the choice of S, because this freedom boils down to a Killing time translation (see Remark 3.1) which has a unique analytic continuation to M^c_R. It is also unnecessary for S to be a Cauchy surface at this stage. Note that in the standard stationary case there is more freedom to choose canonical time coordinates, so it would be unclear whether an analogous construction can be made independent of the choice of such a coordinate. Besides, any cross terms $w \otimes dt$ in the metric would spoil the real-valuedness of the restriction g_R of the analytically continued metric, so it would not be Riemannian.

Whereas the Killing time coordinate on M is used to define the complexifications M^c_R and the Riemannian manifolds M_R, it may be a bad choice of coordinate to analyze the behavior near the edge of S. This will be the case e.g. if M is the right wedge of a static black hole space–time with a bifurcate Killing horizon and we wish to study the behavior near the bifurcation surface.[d] Anticipating these problems we now consider Gaussian normal coordinates near S, instead of the Killing time coordinate, and we study the properties of the complexification procedure above with respect to these new coordinates.

Proposition 3.3. *Let M be a standard static space–time, let $R > 0$ and let x^i denote local coordinates on a portion U of S. Let $x = (x^0, x^i)$ be the corresponding Gaussian normal coordinates on a portion of M, containing U, and let*

[d]This setting will be studied in detail in a forthcoming publication.[9]

$x' = ((x')^0, x^i)$ be Gaussian normal coordinates on a portion of M_R, containing U. We may express the metrics g and g_R in these coordinates as

$$g = -(dx^0)^{\otimes 2} + h_{ij} dx^i dx^j \,, \quad g_R = (d(x')^0)^{\otimes 2} + h'_{ij} dx^i \, dx^j$$

and we then have for all $n \geq 0$:

$$\partial_0^{2n} h_{ij}\big|_U = (-1)^n (\partial'_0)^{2n} h'_{ij}\big|_U \,, \quad \partial_0^{2n+1} h_{ij}\big|_U = 0 = (\partial'_0)^{2n+1} h'_{ij}\big|_U \,. \qquad (3.1)$$

In the ultra-static case we have $x^0 = t$, which means that the metric g is real-analytic in x^0 and its analytic continuation satisfies $g_{ab}(ix^0, x^i) = (g_R)_{ab}(x^0, x^i)$. This immediately implies Eq. (3.1), by the Cauchy–Riemann equations and the reality of g and g_R. In the general case, the Proposition can be interpreted as saying that g is "infinitesimally holomorphic" in $z := x^0 + i(x')^0$.

Proof. The form of the metrics follows from the construction of Gaussian normal coordinates, as is well known.[32] The idea is now to use the fact that the geometries of M and M_R are entirely determined by (S, h, N). The number of coefficients in (h_{ij}, ξ^a) equals $\frac{d(d+1)}{2}$, which is exactly the number of components of Killing's equation. We may write out Killing's equation in the chosen local coordinates, for which the Christoffel symbol vanishes when two or more indices are 0. The (00)-component of Killing's equation is then $\partial_0 \xi^0 = 0$, which means that $\xi^0(x) = N(x^i)$. Substituting this back in the remaining equations yields[e]

$$h_{ij} \partial_0 \xi^j = \partial_i N \,, \quad N \partial_0 h_{ij} = -2 h_{k(i} \partial_{j)} \xi^k - \xi^k \partial_k h_{ij} \,.$$

All normal derivatives of ξ^i and h_{ij} are uniquely determined by the initial data, as can be shown by induction, taking successive normal derivatives of the equations above. In the Riemannian case we find similarly $\xi_R^0(x') = N(x^i)$ and

$$h'_{ij} \partial'_0 \xi_R^j = -\partial'_i N \,, \quad N \partial'_0 h'_{ij} = -2 h'_{k(i} \partial'_{j)} \xi_R^k - \xi_R^k \partial'_k h'_{ij} \,.$$

Note the change of sign in the first equation when compared to the Lorentzian case.

One now proves by induction on $n \geq 0$ that[f]

$$\partial_0^n h_{ij}\big|_U = i^n (\partial'_0)^n h'_{ij}\big|_U \,, \quad \partial_0^n \xi^i\big|_U = i^{n+1} (\partial'_0)^n \xi_R^i\big|_U \,.$$

For $n = 0$, these equalities are true, because they just express the equality of the initial data. (Note in particular that $\xi^i|_U = 0 = \xi_R^i\big|_U$.) Now suppose they hold true

[e] In these coordinates it is less clear that the Cauchy problem is well posed, unless the initial data are analytic, in which case the Cauchy–Kowalewsky Theorem applies.[32] However, we know that the data (Σ, h, N) determine a unique, smooth solution, which is easily written down in adapted coordinates.

[f] The vanishing of the odd normal derivatives on Σ can also be seen by a symmetry argument involving a reflection in the Killing time around the Cauchy surface.

for all $0 \leq l \leq n$. We use Killing's equation and $\partial_0 N = \partial'_0 N = 0$ to compute

$$\begin{aligned}\partial_0^{n+1} h_{ij}\big|_U &= -N^{-1}\partial_0^n \Big(2h_{k(i}\partial_{j)}\xi^k + \xi^k \partial_k h_{ij}\Big)\Big|_U \\ &= -i^{n+1} N^{-1}(\partial'_0)^n \Big(2h'_{k(i}\partial'_{j)}\xi^k_R + \xi^k_R \partial'_k h'_{ik}\Big)\Big|_U \\ &= i^{n+1}(\partial'_0)^{n+1} h'_{ij}\big|_U ,\end{aligned}$$

where the induction hypothesis was used in the second equality. Similarly, by the binomial formula,

$$h_{ij}\partial_0^{n+1}\xi^j\big|_U = -\sum_{l=0}^{n-1}\binom{n}{l}\partial_0^{n-l}h_{ij}\cdot\partial_0^{l+1}\xi^j\Big|_U = i^{n+2}h_{ij}(\partial'_0)^{n+1}\xi^j_R\big|_U ,$$

where we used the fact that, as h_{ij} is invertible, the result for $n+1$ follows, completing the proof by induction. The statement of the proposition is then immediately clear, because both h_{ij} and h'_{ij} are real-valued. □

Corollary 3.1. *For a smooth curve* $\gamma\colon [0,1] \to S$ *the following are equivalent*:

(i) γ *is a geodesic in* (S, h),
(ii) γ *is a geodesic in* M,
(iii) γ *is a geodesic in* M_R.

Proof. We express the geodesic equation in M in terms of local coordinates x^i on S and a Gaussian normal coordinate x^0 near $S \subset M$. Using the notation $\gamma^a := x^a \circ \gamma$, with $\gamma^0 = 0$, the components

$$\partial_s^2\gamma^i = -\Gamma^i{}_{ab}\partial_s\gamma^a\partial_s\gamma^b = -\Gamma^i{}_{jk}\partial_s\gamma^j\partial_s\gamma^k$$

form exactly the geodesic equation in (S, h). The remaining equation is

$$0 = \partial_s^2\gamma^0 = -\Gamma^0{}_{ij}\partial_s\gamma^i\partial_s\gamma^j = \frac{-1}{2}\partial_0 h_{ij}\Big|_U \partial_s\gamma^i\partial_s\gamma^j ,$$

which is true by Proposition 3.3. This proves the equivalence of the first and second statements. The equivalence of the first and third statement is shown in a similar manner. □

4. The Linear Scalar Quantum Field

It is well understood how to quantize a linear real scalar field on any globally hyperbolic space–time.[1–4] In this section we will present this quantization, with a special focus on the case where the space–time is stationary.[7] This extra structure allows one to obtain additional results concerning e.g. ground states for the Killing flow.

As a matter of convention we will identify distributions on M, M_R and Σ with distribution densities, using the natural volume forms determined by the metrics. To unburden our notation we will often leave the volume form implicit, which should not lead to any confusion. However, we point out that the volume form is important when restricting to submanifolds, because in that case a change in volume form is involved. We will also make use of the natural Hilbert spaces of square-integrable functions on the various space–times and Riemannian manifolds, where integration is performed with respect to the volume forms determined by the metrics. This being understood we may leave the volume forms implicit in our notation, writing e.g. $L^2(M)$, $L^2(\Sigma)$ instead of $L^2(M, d\,\mathrm{vol}_g)$ and $L^2(\Sigma, d\,\mathrm{vol}_h)$.

4.1. *The classical scalar field in stationary space–times*

The classical theory of a linear scalar field on a space–time M is described by the (modified) Klein–Gordon equation for $\phi \in C^\infty(M)$,

$$K\phi := (-\Box + V)\phi = 0\,, \tag{4.1}$$

where $\Box := \nabla^a\nabla_a$ denotes the Laplace–Beltrami operator and the potential V is a smooth, real-valued function. V is often chosen to be of the form

$$V = cR + m^2\,, \quad m \geq 0\,, \quad c \in \mathbb{R}$$

with mass m and scalar curvature coupling c. In any globally hyperbolic space–time, the Klein–Gordon equation has a well posed initial value formulation (see e.g. Ref. 2, Chap. 3, Theorem 3). To formulate it we introduce the space of initial data

$$\mathcal{D}(\Sigma) := C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma)\,,$$

as a topological direct sum, where each summand carries the test-function topology.

Theorem 4.1. *Let $\Sigma \subset M$ be a Cauchy surface in a globally hyperbolic space–time M with future pointing normal vector field n^a. For each $(\phi_0, \phi_1) \in \mathcal{D}(\Sigma)$ there is a unique $\phi \in C^\infty(M)$ such that*

$$K\phi = 0\,, \quad \phi|_\Sigma = \phi_0\,, \quad n^a\nabla_a\phi|_\Sigma = \phi_1\,. \tag{4.2}$$

Moreover, $\mathrm{supp}(\phi) \subset J(\mathrm{supp}(\phi_0) \cup \mathrm{supp}(\phi_1))$ *and the linear map $S : \mathcal{D}(\Sigma) \to C^\infty(M)$ which sends (ϕ_0, ϕ_1) to the corresponding solution ϕ of Eq.* (4.2) *is continuous, if $C^\infty(\Sigma)$ is endowed with the usual Fréchet topology.*

It follows from Theorem 4.1 that the Klein–Gordon operator K has unique advanced $(-)$ and retarded $(+)$ fundamental solutions $E^\pm$ and we define $E := E^- - E^+$.

The solution map S and the operator E will be used frequently to translate between the space–time and the initial data formulations of the theory and we note that

$$\begin{aligned} E(f, f') &:= \int_M fEf' := \int_{M^{\times 2}} d\,\mathrm{vol}_g(x) d\,\mathrm{vol}_g(x') f(x) E(x, x') f'(x') \\ &= \int_\Sigma Ef \cdot n^a\nabla_a Ef' - n^a\nabla_a Ef \cdot Ef'\,, \end{aligned} \tag{4.3}$$

where $\Sigma \subset M$ is any Cauchy surface and $f,\ f' \in C_0^\infty(M)$. The kernel of E, acting on $C_0^\infty(M)$, is exactly[1] $KC_0^\infty(M)$ and for later use we introduce the real-linear space

$$L := C_0^\infty(M,\mathbb{R})/KC_0^\infty(M,\mathbb{R})\,.$$

In a stationary, globally hyperbolic space–time (M,ξ), the Killing vector field determines a natural time evolution. We fix a Cauchy surface $\Sigma \subset M$ and use it to write M as a standard stationary space–time (cf. Subsec. 3.1). We will work throughout in adapted coordinates $x^a = (t, x^i)$ and assume that the potential V is stationary,

$$\xi^a \nabla_a V = \partial_0 V = 0\,.$$

As the potential V is real-valued we may view K as a symmetric operator on the dense domain $C_0^\infty(M)$ in $L^2(M)$. We will now separate off the canonical time dependence of this operator and write the spatial dependence in terms of h_{ij}, N, N^i and V. The cleanest way to do so is by ensuring that we obtain symmetric operators in $L^2(\Sigma)$ for the spatial parts. For this reason it is convenient to consider the unitary isomorphism

$$U : L^2(M) \to L^2(\mathbb{R}) \otimes L^2(\Sigma) : f \mapsto \sqrt{N} f$$

onto the Hilbert tensor product, where $\mathbb{R}$ is viewed as a Riemannian manifold with the standard metric dt. To see that U is indeed an isomorphism we use Schwartz Kernels Theorem, the diffeomorphism $M \simeq \mathbb{R} \times \Sigma$ and the fact that $\det g = -N^2 \det h$ and $d\,\mathrm{vol}_g = N dt\, d\,\mathrm{vol}_h$, which may be seen by choosing local coordinates on Σ that diagonalize h_{ij} at a point. The symmetric operator $UNKNU^{-1}$ can now be written as

$$\begin{aligned} N^{\frac{3}{2}} K N^{\frac{1}{2}} &= N^{\frac{3}{2}}(-\Box + V)N^{\frac{1}{2}} \\ &= \partial_0^2 - \left(\nabla_i^{(h)} N^i + N^i \nabla_i^{(h)}\right)\partial_0 \\ &\quad - N^{\frac{1}{2}} \nabla_i^{(h)} (N h^{ij} - N^{-1} N^i N^j) \nabla_j^{(h)} N^{\frac{1}{2}} + V N^2\,. \end{aligned} \tag{4.4}$$

The computation that leads to this expression has been omitted, because it is straightforward.[g]

[g]Instead of the Riemannian manifold (Σ, h) one may also consider $(\Sigma, \tilde{h})$, cf. Theorem 3.1. In this case the unitary map takes the form $U : f \mapsto v^{\frac{d}{2}} f$ and

$$\begin{aligned} v^{\frac{d}{2}} N K N v^{-\frac{d}{2}} &= \partial_0^2 - \left(\nabla_i^{(\tilde{h})} N^i + N^i \nabla_i^{(\tilde{h})}\right)\partial_0 - N \nabla_i^{(\tilde{h})} v^{-2} \tilde{h}^{ij} \nabla_j^{(\tilde{h})} N \\ &\quad + N^2 v^{-4} \frac{d}{2}\left(v(\Box_{\tilde{h}} v) + \frac{d-6}{2} \tilde{h}^{ij} \left(\nabla_i^{(\tilde{h})} v\right)\left(\nabla_j^{(\tilde{h})} v\right)\right) + V N^2\,. \end{aligned}$$

Although the metric $\tilde{h}$ has the advantage of being complete, it may be a less natural choice than h, especially when the space–time M is isometrically embedded into a larger space–time.

Because ξ is a Killing field, the flow Ξ_t preserves the Klein–Gordon equation: $K\Xi_t^*\phi = \Xi_t^*(K\phi)$ for all $t \in \mathbb{R}$. Moreover, if $K\phi = 0$ and ϕ has compactly supported initial data on some Cauchy surface, then the same is true for $\Xi_t^*\phi$. This means that the time flow determines a time evolution on the initial data in $\mathcal{D}(\Sigma)$. Indeed, let S be the solution operator of Theorem 4.1 and let S^{-1} be its inverse, i.e. $S^{-1}(\phi) = (\phi|_\Sigma, n^a\nabla_a\phi|_\Sigma)$. We may define the time evolution maps T_t on $\mathcal{D}(\Sigma)$ by $T_t := S^{-1}\Xi_t^*S$. The maps T_t form a continuous (even smooth) one-parameter group for $t \in \mathbb{R}$, by Theorem 4.1. The infinitesimal generator H_{cl} of the group T_t is the classical Hamiltonian:

Lemma 4.1. *The* (*classical*) *Hamiltonian operator* H_{cl} *is given* (*in matrix notation on* $\mathcal{D}(\Sigma)$) *by*

$$\begin{aligned} H_{\mathrm{cl}}\begin{pmatrix}\phi_0\\ \phi_1\end{pmatrix} &:= -i\partial_t T_t \begin{pmatrix}\phi_0\\ \phi_1\end{pmatrix}\bigg|_{t=0} \\ &= -i\begin{pmatrix} N^i\nabla_i^{(h)} & N \\ \nabla_i^{(h)}Nh^{ij}\nabla_j^{(h)} - VN & \nabla_i^{(h)}N^i \end{pmatrix}\begin{pmatrix}\phi_0\\ \phi_1\end{pmatrix}. \end{aligned}$$

Proof. The computation is simplified somewhat by defining $X := \begin{pmatrix} I & 0 \\ N^i\nabla_i^{(h)} & N\end{pmatrix}$, with inverse $X^{-1} := N^{-1}\begin{pmatrix} N & 0 \\ -N^i\nabla_i^{(h)} & I\end{pmatrix}$. Note that $X\begin{pmatrix}\phi_0\\ \phi_1\end{pmatrix} = \begin{pmatrix}\phi_0\\ \partial_0\phi|_\Sigma\end{pmatrix}$, where $\phi := S(\phi_0,\phi_1)$. Now the first row of $XH_{\mathrm{cl}}X^{-1}$ is simply $(0\ \ -iI)$ and the second row can be found by writing $\partial_0^2 = N^{\frac{1}{2}}\partial_0^2 N^{-\frac{1}{2}}$ and by eliminating the second-order time derivative using Eq. (4.4) and $K\phi = 0$. H_{cl} is then obtained from a straightforward matrix multiplication. The details are omitted. □

For any solution $\phi \in C^\infty(M)$ of the Klein–Gordon equation one defines the stress-energy–momentum tensor

$$T_{ab}(\phi) := \nabla_{(a}\bar{\phi}\nabla_{b)}\phi - \frac{1}{2}g_{ab}\left(\nabla^c\bar{\phi}\nabla_c\phi + V|\phi|^2\right),$$

which is symmetric and

$$\nabla^a T_{ab}(\phi) = \frac{-1}{2}(\nabla_b V)|\phi|^2\,,$$

because $K\phi = 0$. By Killing's equation, $\nabla^a\xi^b$ is antisymmetric, so the energy–momentum one-form

$$P_a(\phi) := \xi^b T_{ab}(\phi)$$

satisfies

$$\nabla^a P_a(\phi) = \xi^b\nabla^a(T_{ab}(\phi)) = \frac{-1}{2}(\partial_0 V)|\phi|^2 = 0\,,$$

where we used the assumption that V is stationary. Note that energy–momentum is conserved, even though the stress–tensor may not be divergence free. On a Cauchy surface Σ with future pointing normal n^a, the energy density is defined by

$$\varepsilon_\Sigma(\phi) := n^a P_a(\phi)|_\Sigma = n^a \xi^b T_{ab}(\phi)|_\Sigma \,.$$

If $\phi = S(\phi_0, \phi_1)$ for some $(\phi_0, \phi_1) \in \mathcal{D}(\Sigma)$, then we can also define the total energy on Σ by

$$\mathcal{E}(\phi) := \int_\Sigma \varepsilon_\Sigma(\phi) \,.$$

The conservation of $P_a(\phi)$ implies that $\mathcal{E}(\phi)$ is independent of the choice of Cauchy surface, by Stokes' Theorem. In particular, $\mathcal{E}(\Xi_t^* \phi) = \mathcal{E}(\phi)$ for all t, because the left-hand side is the integral of $\varepsilon_{\Sigma'}(\phi)$ over the Cauchy surface $\Sigma' := \Xi_t(\Sigma)$.

Lemma 4.2. *Viewing $\mathcal{D}(\Sigma)$ as a dense domain in $L^2(\Sigma)^{\oplus 2}$ we have*

$$\mathcal{E}(S(\phi_0, \phi_1)) = \langle (\phi_0, \phi_1), A(\phi_0, \phi_1) \rangle \,,$$

where the operator A is given by

$$A := \frac{1}{2} \begin{pmatrix} -\nabla_i^{(h)} N h^{ij} \nabla_j^{(h)} + VN & -\nabla_i^{(h)} N^i \\ N^i \nabla_i^{(h)} & N \end{pmatrix}.$$

In particular, $A = \frac{i}{2} \sigma H_{\mathrm{cl}}$ with $\sigma := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and $A \geq \frac{1}{2} \begin{pmatrix} VN & 0 \\ 0 & N^{-1} v^2 \end{pmatrix}$.

Proof. The form of $\mathcal{E}$ can be computed by expressing the energy density on Σ in terms of the initial data. The computation is straightforward, so the details are omitted. The final equality is then obvious from Lemma 4.1, whereas the final inequality follows from

$$\begin{aligned} \langle (\phi_0, \phi_1), A(\phi_0, \phi_1) \rangle = \frac{1}{2} \int_\Sigma & N h^{ij} \left(\nabla_i^{(h)} \overline{\phi_0} + N^{-1} N_i \overline{\phi_1} \right) \left(\nabla_j^{(h)} \phi_0 + N^{-1} N_j \phi_1 \right) \\ & + VN |\phi_0|^2 + (N - N^{-1} N^i N_i) |\phi_1|^2 \,, \end{aligned}$$

where the first term in the integrand is nonnegative and may be dropped. $\square$

When $V > 0$ everywhere, we may define an energetic inner product on $L \otimes \mathbb{C}$ by setting

$$\langle f, f' \rangle_e := \langle S^{-1} E f, A S^{-1} E f' \rangle \,,$$

where the inner product on the right-hand side is in $L^2(\Sigma)^{\oplus 2}$. Note that $\langle \, , \rangle_e$ is indeed positive and nondegenerate, by the properties of A established in Lemma 4.2 and the positivity of VN and $N^{-1} v^2$. Since V is stationary, the energetic inner product is independent of the choice of Cauchy surface, like the energy, because

$$\| f \|_e^2 = \mathcal{E}(Ef) \,.$$

Definition 4.1. When V is stationary and $V>0$, the *energetic Hilbert space* $\mathcal{H}_e$ is the Hilbert space completion of $L\otimes\mathbb{C}$ in the energetic norm.

$\mathcal{H}_e$ can be interpreted as the space of all (complex) finite energy solutions of the Klein–Gordon equation (4.1).

The following detailed description of the energetic Hilbert space is the main result of this section. The proof makes use of strictly positive operators and we have collected some basic results on such operators in the Appendix (see also Ref. 38).

Theorem 4.2. *Let M be a stationary, globally hyperbolic space–time with a Cauchy surface Σ and assume that V is stationary and $V>0$. Let $\hat{A}$ denote the Friedrichs extension of the operator A of Lemma 4.2. The linear map $q_{\mathrm{cl}}:\mathcal{D}(\Sigma)\to L^2(\Sigma)^{\oplus 2}$ defined by $q_{\mathrm{cl}}(\phi_0,\phi_1):=\sqrt{\hat{A}}\binom{\phi_0}{\phi_1}$ is continuous, injective, has dense range, commutes with complex conjugation and satisfies $\|q_{\mathrm{cl}}(\phi_0,\phi_1)\|^2=\mathcal{E}(S(\phi_0,\phi_1))$. Hence, $\mathcal{H}_e\simeq L^2(\Sigma)^{\oplus 2}$.*

There is a unique, strongly continuous unitary group $O_t=e^{itH_e}$ on $L^2(\Sigma)^{\oplus 2}$ such that $O_tq_{\mathrm{cl}}=q_{\mathrm{cl}}T_t$. Its infinitesimal generator is given by $H_e:=2i\sqrt{\hat{A}}\sigma\sqrt{\hat{A}}$. iH_e commutes with complex conjugation, H_e and all its powers H_e^n, $n\in\mathbb{N}$, are essentially self-adjoint on the range of q_{cl}, H_e is invertible and the range of q_{cl} is a core for $|H_e|^{-1}$.

The explicit characterization of $\mathcal{H}_e$ in terms of $L^2(\Sigma)^{\oplus 2}$ is often very useful, although it is less aesthetically appealing, because it requires the choice of an arbitrary Cauchy surface Σ.

Proof. We first consider the Friedrichs extension $\hat{A}$ of A, which is a positive, self-adjoint operator. By Lemma A.7, $\mathcal{D}(\Sigma)$ is a core for $\hat{A}^{\frac{1}{2}}$. Furthermore, $\hat{A}\geq B$, where the operator $B:=\frac{1}{2}\begin{pmatrix}VN & 0\\ 0 & N^{-1}v^2\end{pmatrix}$ is defined on $\mathcal{D}(\Sigma)$ (cf. Lemma 4.2). Note that B is essentially self-adjoint with a strictly positive closure, by Proposition A.1. Hence, $\hat{A}$ is also strictly positive, by Lemma A.6 and $\mathcal{D}(\Sigma)$ is in the domain of $\hat{A}^{-\frac{1}{2}}$. Moreover, as $\mathcal{D}(\Sigma)$ is a core for $\hat{A}^{\frac{1}{2}}$, the latter has a dense range on $\mathcal{D}(\Sigma)$. Therefore, q_{cl} is a well defined, injective linear map with dense range $\mathcal{R}$ and by Lemma 4.2, $\|q_{\mathrm{cl}}(\phi_0,\phi_1)\|^2=\mathcal{E}(S(\phi_0,\phi_1))$. As S is continuous, the last equation also entails the continuity of q_{cl}. (Alternatively one may use Theorem A.1 of the Appendix.) Also note that A commutes with complex conjugation in $L^2(\Sigma)^{\oplus 2}$, hence the same is true for $\hat{A}^{\frac{1}{2}}$ and for q_{cl}.

Because q_{cl} is invertible we may define O_t by $O_t=q_{\mathrm{cl}}T_tq_{\mathrm{cl}}^{-1}$ on $\mathcal{R}$. Note that the total energy $\|O_tq_{\mathrm{cl}}(\phi_0,\phi_1)\|^2=\mathcal{E}(\Xi_t^*S(\phi_0,\phi_1))$ is independent of t, so each O_t is a densely defined isometry, which extends uniquely to a unitary isomorphism on the entire Hilbert space, again denoted by O_t. $O_t^{-1}=O_{-t}$ and the continuity of $f\mapsto T_tf$ in the test-function topology entails the strong continuity of O_t.

Because the time-derivative of $T_t(\phi_0,\phi_1)$ converges in the test-function topology of $\mathcal{D}(\Sigma)$ and q_{cl} is continuous, the infinitesimal generator of O_t is well defined on the range $\mathcal{R}$ of $q_{\rm cl}$, where it is given by

$$H_e = q_{\rm cl} H_{\rm cl} q_{\rm cl}^{-1} = 2i\sqrt{\hat{A}}\sigma\sqrt{\hat{A}}\,,$$

because of the Lemmas 4.1 and 4.2. Both H_e and O_t preserve $\mathcal{R}$, so H_e and all its powers are essentially self-adjoint on $\mathcal{R}$ by Lemma 2.1 in Ref. 39.

$\hat{A}$ commutes with complex conjugation, so it is clear that iH_e also commutes with it. Furthermore, the map $M := \frac{i}{2}\hat{A}^{-\frac{1}{2}}\sigma\hat{A}^{-\frac{1}{2}}$ is well defined on $\mathcal{R}$ and it satisfies $MH_e = I$ there. Note that M is closable, because it is symmetric and densely defined. By Lemma A.1, H_e must be invertible. Lemma A.4 implies that H_e^{-1} is self-adjoint and invertible and a core is given by $H_e\mathcal{R} \subset \mathcal{R}$. As M is a symmetric extension of H_e^{-1} on this domain, we must have $\bar{M} = H_e^{-1}$ and the domain $\mathcal{R}$ of M is a core for H_e^{-1} and hence also for $|H_e|^{-1}$, by the Spectral Calculus Theorem. □

4.2. *The scalar quantum field in stationary space–times and equilibrium one-particle structures*

We now study the quantized scalar field in a stationary space–time, where the ground states play a similarly important role for the theory as the vacuum state in Minkowski space–time. Because of the importance of quasi-free equilibrium states (cf. Sec. 2) we first focus on equilibrium one-particle structures, whereas the ground and equilibrium states (beyond their two-point distributions) will be discussed in Sec. 5 below.

The well posedness of the Cauchy problem established in Theorem 4.1 remains true if we specify arbitrary distributional initial data, allowing distributional solutions and using distributional topologies.[40] In this setting it is natural to introduce local observables, associated to arbitrary $f \in C_0^\infty(M)$, which measure the distributional field ϕ by the formula $\phi(f) := \int \phi f$. These observables $\phi \mapsto \phi(f)$ can be regarded as functions on the space of classical solutions ϕ and we may use them to generate an algebra of observables. We choose to work with the Weyl C^*-algebra $\mathcal{W}^{\rm cl} := \mathcal{W}(L, 0)$, whose elements we interpret as $e^{i\phi(f)}$, which remains bounded when ϕ and f are real-valued.

Interpreting the right-hand side of Eq. (4.3) in terms of initial values and momenta motivates the introduction of the symplectic space (L, E), so that the corresponding quantum theory is described by $\mathcal{W} := \mathcal{W}(L, E)$. For each open subset $O \subset M$ we will denote by $\mathcal{W}(O)$ the C^*-subalgebra generated by those $W(f)$ with f supported in O (and similarly for $\mathcal{W}^{\rm cl}(O)$). In this way one obtains a net of local C^*-algebras.[4,41]

When (M, ξ) is a stationary, globally hyperbolic space–time and V is stationary, $(L, 0, T_{-t})$ and (L, E, T_{-t}) become one-particle dynamical systems. This follows from the fact that Ξ^*_{-t} preserves the metric and that the $E^\pm$ are unique, so the symplectic form $E(f, f') := \int_M fEf'$ is preserved. We may consider the associated quasi-free dynamical systems $\left(\mathcal{W}^{\mathrm{cl}}, \alpha_t^{\mathrm{cl}}\right)$ and $(\mathcal{W}, \alpha_t)$, so that

$$\alpha_t^{\mathrm{cl}}(W(f)) = W(\Xi_{-t}^* f)\,, \quad \alpha_t(W(f)) = W(\Xi_{-t}^* f)$$

for all $f \in L$.[h] α_t^{cl} and α_t describe the Killing time flow at an algebraic level and we note that $\alpha_t(\mathcal{W}(O)) = \mathcal{W}(\Xi_t(O))$ and similarly in the classical case. However, neither α_t^{cl} nor α_t is norm-continuous in t, as $\|w(f) - w(g)\| = 2$ for all $f \neq g \in L$ (Ref. 19, Proposition 3.10). For this reason, general results on C^*-dynamical systems[14,20] do not apply directly to our situation. (Nor can we view $(\mathcal{W}, \alpha_t)$ as a W^*-dynamical system, because $\mathcal{W}$ is not a W^*-algebra or von Neumann algebra.)

In order to take advantage of the smoothness of the time evolution maps T_t on $\mathcal{D}(\Sigma)$ we need the following definition.

Definition 4.2. We call a state ω on the Weyl C^*-algebra $\mathcal{W}$ (or $\mathcal{W}^{\mathrm{cl}}$) D^k, $k > 0$, when it is C^k (cf. Definition 2.6) and the maps

$$\omega_n(f_1, \ldots, f_n) := (-i)^n \partial_{s_1} \cdots \partial_{s_n} \omega(W(s_1 f_1) \cdots W(s_n f_n))|_{s_1 = \cdots = s_n = 0}$$

are *distributions* on $M^{\times n}$ for all $1 \leq n \leq k$. The ω_n are called the n-point distributions. A state is called *regular*, or D^∞, when it is D^k for all $k > 0$.

In our setting the distributional character of the ω_n is natural and useful.

Remark 4.1. An alternative description of the scalar quantum field uses the *-algebra $\mathcal{A}$, generated by the identity I and the smeared field operators $\Phi(f)$, $f \in C_0^\infty(M)$, satisfying

(i) $f \mapsto \Phi(f)$ is $\mathbb{C}$-linear,
(ii) $\Phi(f)^* = \Phi(\bar{f})$,
(iii) $K\Phi(f) := \Phi(Kf) = 0$,
(iv) $[\Phi(f), \Phi(f')] = iE(f, f')I$.

Although the algebras $\mathcal{A}$ and $\mathcal{W}$ are technically different, their relation can be understood from a physical point of view by formally setting $W(f) = e^{i\Phi(f)}$. In suitable representations this can be made rigorous. This applies in particular to regular states ω on $\mathcal{W}$, which give rise to a corresponding state on $\mathcal{A}$.

4.2.1. *Two-point distributions*

When ω is a D^2 state on $\mathcal{W}$, we may identify the one-particle structure $(p, \mathcal{K})$ of ω_2 as a map into a subspace of the GNS-representation space $\mathcal{H}_\omega$, as in the proof of Proposition 2.3. A similar construction applies to the so-called truncated two-point distribution, $\omega_2^T(x, x') := \omega_2(x, x') - \omega_1(x)\omega_1(x')$, where we now take $p(f) := \pi_\omega(\Phi(f) - \omega_1(f)I)\Omega_\omega$. Note that ω_2^T is indeed a two-point distribution,

[h]The sign in T_{-t} is explained by the desire to have $\alpha_t^{\mathrm{cl}}\phi = \Xi_t^*\phi$ for the field ϕ, so that $\alpha_t^{\mathrm{cl}}(\phi(f)) = (\Xi_t^*\phi)(f) = \phi(\Xi_{-t}^* f)$ in the distributional perspective. The same argument applies to the quantum case.

(cf. Theorem 2.3) and that $\omega_2 = \omega_2^T$ when $\omega_1 = 0$, so in that case the two constructions coincide.

When ω_2 is a distribution, the associated one-particle structure can be viewed as a $\mathcal{K}$-valued distribution p which satisfies the Klein–Gordon equation.[42] (Conversely, when p is a distribution, the associated ω_2 is also a distribution.) For any Cauchy surface Σ, p is uniquely determined by its initial data, which form a continuous linear map $q_\Sigma : \mathcal{D}(\Sigma) \to \mathcal{K}$ with dense range and such that

$$\left\langle q_\Sigma(\overline{\phi_0}, \overline{\phi_1}), q_\Sigma(\phi_0', \phi_1')\right\rangle - \left\langle q_\Sigma(\overline{\phi_0'}, \overline{\phi_1'}), q_\Sigma(\phi_0, \phi_1)\right\rangle = i \int_\Sigma \phi_0\phi_1' - \phi_1\phi_0'$$

(cf. Eq. (4.3)). Conversely, any such linear map q_Σ determines a unique one-particle structure. Indeed, just like smooth solutions to the Klein–Gordon equation, two-point distributions are uniquely determined by their initial data on a Cauchy surface:

Proposition 4.1. *Let $\Sigma \subset M$ be a Cauchy surface in a globally hyperbolic space–time with future pointing normal n^a and let ω be a distribution density in $M^{\times 2}$. If $K_x\omega(x,y) = K_y\omega(x,y) = 0$, then the restrictions*

$$\omega_{ij} := (n^a\nabla_a)^i_x(n^b\nabla_b)^j_y\omega\big|_{\Sigma^{\times 2}}\,,$$

are well defined distribution densities in $\Sigma^{\times 2}$ for all i, $j \in \mathbb{N}$.

Conversely, for any four distribution densities ω_{ij}, $0 \le i, j \le 1$, on $\Sigma^{\times 2}$, there is a unique distribution density ω on $M^{\times 2}$ such that

$$K_x\omega = K_y\omega = 0\,, \quad (n^a\nabla_a)^i_x(n^b\nabla_b)^j_y\omega\big|_{\Sigma^{\times 2}} = \omega_{ij}\,. \tag{4.5}$$

Support and continuity properties analogous to Theorem 4.1 also hold, but we will not need them. We omit the proof of this basic result.

There is a preferred class of D^2 states, called Hadamard states, which are characterized by the fact that their two-point distribution has a singularity structure that is of the same form as for the Minkowski vacuum state. These states are important, because the renormalized Wick powers and stress tensor of the quantum field have finite expectation values in them. To put it more precisely, ω_2 is of Hadamard form if and only if[43]

$$\begin{aligned} WF(\omega_2) = \{(x,k;y,l) \in T^*M^{\times 2} \mid\ & l \neq 0 \text{ is future pointing and} \\ & \text{light-like and } (y,l) \text{ generates a geodesic } \gamma \text{ which} \\ & \text{goes through } x \text{ with tangent vector } -k\}\,. \end{aligned} \tag{4.6}$$

This condition is already implied by one of the following apparently weaker, and often more convenient, estimates on ω_2 or its associated one-particle structure $(p, \mathcal{K})$:

$$WF(\omega_2) \subset V^-M \times V^+M\,, \quad WF(p) \subset V^+M\,,$$

where $V^\pm M \subset T^*M$ is the space of future $(+)$ or past $(-)$ pointing causal co-vectors on M (cf. Ref. 42, Proposition 6.1). For any regular state (even if it is not quasi-free) the Hadamard condition allows one to estimate the singularity structure of all higher n-point distributions too,[44] so that the state satisfies the microlocal spectrum condition of Ref. 45.

By the Propagation of Singularities Theorem and the fact that ω_2 solves the Klein–Gordon equation in both variables it suffices to check the condition in Eq. (4.6) on a Cauchy surface Σ:

$$WF(\omega_2)|_\Sigma \subset \{(x,-k;x,k)\,|\,(x,k) \in V^+M|_\Sigma\}\,.$$

Unfortunately it is somewhat complicated to see whether a state ω_2 is Hadamard by inspecting its initial data on a Cauchy surface Σ. The initial data of ω_2 should be smooth away from the diagonal in $\Sigma^{\times 2}$, so it suffices to characterize the singularities on the diagonal. However, for the singularities on the diagonal we are not aware of any argument that avoids the use of the Hadamard parametrix construction, which involves the Hadamard series for which Hadamard states were originally named.

4.2.2. *Equilibrium two-point distributions*

An equilibrium one-particle structure $(p, \mathcal{K})$ has some nice additional structure when p is a distribution:

Lemma 4.3. *If $(p, \mathcal{K})$ is an equilibrium one-particle structure such that p is a distribution, then the unitary group $\tilde{O}_t$ on $\mathcal{K}$ defined by $\tilde{O}_t p = p\Xi^*_{-t}$ (on $C_0^\infty(M)$) is strongly continuous, $\tilde{O}_t = e^{itH}$. Its strong derivative is well defined on the range of p, H is essentially self-adjoint on this range and $Hp(f) = ip(\partial_0 f)$ for all $f \in C_0^\infty(M)$.*

Proof. The strong continuity of $\tilde{O}_t$ follows from the continuity of $t \mapsto \Xi^*_{-t} f$ in the test-function topology and the fact that p is a distribution. The formula for H on the range of p can be deduced from the continuity of p by a direct calculation:

$$Hp(f) := -i\partial_t \tilde{O}_t p(f)|_{t=0} = -i\partial_t p(\Xi^*_{-t}(f))|_{t=0} = ip(\partial_0 f)\,.$$

The essential self-adjointness of H on the range of p then follows from Chernoff's Lemma.[39] □

The next two results are the main results of this section. They are existence and uniqueness results for nondegenerate ground and β-KMS one-particle structures. For the existence of a nondegenerate ground we adapt a result of Ref. 7, which imposed additional restrictions on the potential V and on the Killing field in order to obtain such a ground one-particle structure with, in addition, a mass gap. For the existence of a nondegenerate β-KMS one-particle structure see Refs. 6 and 27.

Theorem 4.3. *Let M be a globally hyperbolic, stationary space–time and consider a linear scalar field with a stationary potential V such that $V > 0$.*

(i) *There exists a nondegenerate ground one-particle structure* $(p_0, \mathcal{K}_0)$, *with* $\mathcal{K}_0 \subset \mathcal{H}_e$ *the closed range of*

$$p_0(f) := \sqrt{2}|H_e|^{-\frac{1}{2}} P_- p_{\mathrm{cl}}(f)\,,$$

where P_- *is the spectral projection onto the negative part of the spectrum of* H_e *and* $p_{\mathrm{cl}}(f) := q_{\mathrm{cl}} S^{-1} E(f)$.

(ii) *For every* $\beta > 0$ *there exists a nondegenerate* β*-KMS one-particle structure* $\big(p_{(\beta)}, \mathcal{K}_{(\beta)}\big)$, *with* $\mathcal{K}_{(\beta)} \subset \mathcal{H}_e^{\oplus 2}$ *the closed range of*

$$\begin{aligned} p_{(\beta)}(f) &= \sqrt{2} P_- |H_e|^{-\frac{1}{2}} \big(I - e^{-\beta|H_e|}\big)^{-\frac{1}{2}} p_{\mathrm{cl}}(f) \\ &\quad \oplus \sqrt{2} P_+ |H_e|^{-\frac{1}{2}} e^{-\frac{\beta}{2}|H_e|} \big(I - e^{-\beta|H_e|}\big)^{-\frac{1}{2}} p_{\mathrm{cl}}(f)\,. \end{aligned}$$

The occurrence of P_-, rather than P_+, is in line with the footnote h on page 31.

Proof. We start with the $\mathcal{H}_e$-valued distribution $p_{\mathrm{cl}}(f) := q_{\mathrm{cl}} S^{-1} E(f)$ and the unitary group O_t determined by Theorem 4.2. Define $p_0(f) := \sqrt{2}|H_e|^{-\frac{1}{2}} P_- p_{\mathrm{cl}}(f)$ and let the closed range of p_0 be denoted by $\mathcal{K}_0$. It is not hard to see that $O_t p_0(f) = p_0(\Xi_t^* f)$, so O_t preserves $\mathcal{K}_0$ and we may let $\tilde{O}_t := O_{-t}|_{\mathcal{K}}$. The generator H of this strongly continuous unitary group is the restriction of $-H_e$, which is strictly positive there. The range of p_0 is in the domain of H and $H^{-\frac{1}{2}}$, by Theorem 4.2. If we let C denote the complex conjugation on $L^2(\Sigma)^{\oplus 2}$, then $CH_eC = -H_e$, so $CP_-C = P_+$, the spectral projection onto the positive part of the spectrum of H_e. Thus,

$$\begin{aligned} \langle p_0(\bar{f}), p_0(f')\rangle &= 2\langle p_{\mathrm{cl}}(\bar{f}), |H_e|^{-1} P_- p_{\mathrm{cl}}(f')\rangle \\ &= -2\langle CH_e^{-1} P_- p_{\mathrm{cl}}(f'), C p_{\mathrm{cl}}(\bar{f})\rangle \\ &= 2\langle H_e^{-1} P_+ p_{\mathrm{cl}}(\overline{f'}), p_{\mathrm{cl}}(f)\rangle \\ &= 2\langle p_{\mathrm{cl}}(\overline{f'}), |H_e|^{-1} P_- p_{\mathrm{cl}}(f)\rangle + 2\langle p_{\mathrm{cl}}(\overline{f'}), H_e^{-1} p_{\mathrm{cl}}(f)\rangle \\ &= \langle p_0(\overline{f'}), p_0(f)\rangle + i\langle S^{-1}E\overline{f'}, \sigma S^{-1} E f\rangle \\ &= \langle p_0(\overline{f'}), p_0(f)\rangle - iE(f, f')\,. \end{aligned}$$

This proves that $(p_0, \mathcal{K}_0)$ is a nondegenerate ground one-particle structure.

The formula for $p_{(\beta)}$ is well defined, because the range of p_{cl} is in the domain of $|H_e|^{-1}$ by Theorem 4.2. It defines a $\mathcal{K}_{(\beta)}$-valued distribution with dense range, which solves the Klein–Gordon equation. Just like for the ground one-particle structure one may check that $\langle p_{(\beta)}(\bar{f}), p_{(\beta)}(f')\rangle - \langle p_{(\beta)}(\overline{f'}), p_{(\beta)}(f)\rangle = iE(f, f')$, so $(p_{(\beta)}, \mathcal{K}_{(\beta)})$ does indeed define a one-particle structure.

Viewing $\mathcal{K}_{(\beta)}$ as a subspace of $\mathcal{H}_e^{\oplus 2}$ we note that $O_t^{\oplus 2}$ preserves the range of $p_{(\beta)}$, because $O_t^{\oplus 2} p_{(\beta)}(f) = p_{(\beta)}(\Xi_t^* f)$. We can therefore define a strongly continuous unitary group $\tilde{O}_t$ on $\mathcal{K}^{(\beta)}$ as the restriction of $O_{-t}^{\oplus 2}$. The generator H of $\tilde{O}_t$ is given by the restriction of $|H_e| \oplus -|H_e|$ and the range of $p_{(\beta)}$ is contained in $D\big(e^{-\frac{\beta}{2}H}\big)$.

One may then compute

$$\begin{aligned}&\left\langle e^{-\frac{\beta}{2}H}p_{(\beta)}(\bar{f}),e^{-\frac{\beta}{2}H}p_{(\beta)}(f')\right\rangle\\&\quad=\left\langle p_{\mathrm{cl}}(\bar{f}),|H_e|^{-1}\big(I-e^{-\beta|H_e|}\big)^{-1}\big(P_+ + e^{-\beta|H_e|}P_-\big)p_{\mathrm{cl}}(f')\right\rangle\\&\quad=\left\langle p_{(\beta)}(\overline{f'}),p_{(\beta)}(f)\right\rangle.\end{aligned}\tag{4.7}$$

This implies the one-particle KMS-condition, because for any $f,\ f'\in C_0^\infty(M,\mathbb{R})$ the function

$$F_{ff'}(z):=\left\langle e^{-\frac{i}{2}\bar{z}H}p_{(\beta)}(\bar{f}),e^{\frac{i}{2}zH}p_{(\beta)}(f')\right\rangle,$$

is bounded and continuous on $\overline{\mathrm{S}_\beta}$ and holomorphic in its interior. The correct boundary conditions follow from Eq. (4.7). $\square$

As $(p_0,\mathcal{K}_0)$ is nondegenerate, the associated quasi-free state is nondegenerate too (Proposition 2.3) and hence it is pure (by Borchers' Theorem 2.1). We then see from Theorem 2.4 that p_0 already has dense range on the real subspace. (Of course a direct proof of this fact is also possible.)

Remark 4.2. Note that there is a connection between the classical energy and the Hamiltonian operator H_0 in the ground one-particle structure, which is given by

$$\langle p_0(f),H_0p_0(f)\rangle+\langle p_0(\bar{f}),H_0p_0(\bar{f})\rangle=2\mathcal{E}(Ef),$$

as may be shown by the same techniques employed in the proof of Theorem 4.3.

Next we establish a uniqueness result for nondegenerate ground and β-KMS one-particle structures.[6,46,i]

Proposition 4.2. *Let* $\left(p_2,\mathcal{K}_2,\tilde{O}_t^{(2)}\right)$ *be a ground, respectively β-KMS, one-particle structure (with $\beta>0$) and let P_2 be the orthogonal projection onto the space of $\tilde{O}_t^{(2)}$-invariant vectors. Let $\left(p_1,\mathcal{K}_1,\tilde{O}_t^{(1)}\right)$ be the nondegenerate ground, respectively β-KMS, one-particle structure of Theorem* 4.3*. Then there is a unique isometry $U:\mathcal{K}_1\to\mathcal{K}_2$ such that $\tilde{O}_t^{(2)}U=U\tilde{O}_t^{(1)}$ and $Up_1=(I-P_2)p_2$. In particular, if $P_2=0$, then U is an isomorphism.*

Let $w:=\omega_2^{(2)}-\omega_2^{(1)}$ denote the difference of the associated two-point functions $\omega_2^{(i)}$. Then w is a real-valued, symmetric (weak) bi-solution to the Klein–Gordon

[i]Our uniqueness result is a slight strengthening of the results of Refs. 6 and 46, in our setting, because our definition of β-KMS one-particle structures is slightly less stringent and we provide a bit more detail on degenerate one-particle structures. Note that Ref. 46 formulates and proves uniqueness in the class of nondegenerate ground one-particle structures, for which p already has a dense range on the real linear space L (which entails that the associated quasi-free ground state is pure by Theorem 2.4). That this extra condition is not needed for the proof was pointed out by the same author in Ref. 6, which also proves uniqueness of nondegenerate β-KMS one-particle structures.

equation which is of positive type and independent of the Killing time (in both entries). If p_2 is a distribution on M, then $w \in C^\infty(M^{\times 2})$.

Proof. The proof follows Ref. 46 (see also Ref. 47). For arbitrary f, $f' \in C_0^\infty(M,\mathbb{R})$ the function

$$\begin{aligned} F(t) &:= \left\langle p_2(f), \tilde{O}_t^{(2)} p_2(f') \right\rangle_{\mathcal{K}_2} - \left\langle p_1(f), \tilde{O}_t^{(1)} p_1(f') \right\rangle_{\mathcal{K}_1} \\ &= \left\langle p_2(f), e^{itH_2} p_2(f') \right\rangle_{\mathcal{K}_2} - \left\langle p_1(f), e^{itH_1} p_1(f') \right\rangle_{\mathcal{K}_1} \end{aligned}$$

is continuous (by the Definition 2.7 of ground and β-KMS one-particle structures) and real-valued on $\mathbb{R}$. Suppose both one-particle structures satisfy the one-particle β-KMS condition at the same $\beta > 0$. There is then a bounded continuous extension $\tilde{F}$ of F to $\overline{\mathrm{S}_\beta}$, holomorphic in the interior. By repeatedly applying Schwarz' reflection principle,[23] $\tilde{F}$ extends to a bounded holomorphic function on all of $\mathbb{C}$, which means that $\tilde{F}$ and F are constant, by Liouville's Theorem.[23] Similarly, if both are ground one-particle structures, the positivity of the infinitesimal generators H_i implies that there is a bounded, holomorphic function F_+ in the upper half plane, which has F as its boundary value. By Schwarz' reflection principle, F_+ can be extended to a bounded holomorphic function on the entire plane, which again means that F is constant.

Note that the range of p_1 is in the domain of H_1, because the strong derivative $\partial_t \tilde{O}_t^{(1)} p_1(f)|_{t=0}$ exists (cf. Theorem 4.3). The same is true for p_2 and H_2, because $\left\| \left(\tilde{O}_t^{(2)} - I \right) p_2(f) \right\|^2 - \left\| \left(\tilde{O}_t^{(1)} - I \right) p_1(f) \right\|^2 \equiv 0$, by the previous paragraph. The constancy of F implies $\partial_t^2 F|_{t=0} = 0$, i.e.

$$\langle p_1(f), H_1^2 p_1(f') \rangle_{\mathcal{K}_1} = \langle p_2(f), H_2^2 p_2(f') \rangle_{\mathcal{K}_2} .$$

This equality must hold for all f, $f' \in C_0^\infty(M)$, by complex (anti-)linearity. We may therefore define linear maps $X_i := H_i p_i$ and we let $V_i := \ker(X_i)$ denote their kernels. By the previous equation, $V_1 = V_2 =: V$, so the X_i descend to linear injections $\tilde{X}_i : C_0^\infty(M)/V \to \mathcal{K}_i$. We set $U := \tilde{X}_2 \tilde{X}_1^{-1}$ between the ranges of the X_i. It is obvious from the previous paragraph that U is an isometry, because $UH_1 p_1 = H_2 p_2$. The nondegeneracy of the first one-particle structure implies that H_1 is injective, while the range of p_1 is a core for it. It follows that the map $\tilde{X}_1$ has a dense range, so U extends by continuity to an isometry from $\mathcal{K}_1$ into $\mathcal{K}_2$. Note that U intertwines between the unitary groups, because $\tilde{O}_t^{(i)} H_i p_i(f) = H_i p_i(\Xi_{-t}^* f)$. Hence $UH_1 = H_2 U$ and $P_2 U H_1 = (P_2 H_2) U = 0$, which means that $P_2 U = 0$, because H_1 has a dense range. Let R be the unique linear map such that $RP_2 = 0$ and $RH_2 = I - P_2$. Then $U = RH_2 U = RUH_1$ and $Up_1 = RUH_1 p_1 = RH_2 p_2 = (I - P_2) p_2$. The uniqueness of U is then obvious, as p_1 has a dense range.

By construction, $w := \omega_2^{(2)} - \omega_2^{(1)}$ is a real-valued, symmetric bi-solution to the Klein–Gordon equation (in a weak sense). Moreover, as U is isometric and

$Up_1 = (I - P_2)p_2$,

$$w(\bar{f}, f) = \|p_2(f)\|^2 - \|Up_1(f)\|^2 = \|P_2 p_2(f)\|^2 \geq 0\,,$$

so w is of positive type. For fixed $f, f' \in C_0^\infty(M)$, $w(\bar{f}, \Xi^*_{-t} f') = F(t) = w(\overline{\Xi^*_t f}, f')$ is constant, as we saw in the first paragraph of this proof. If p_2 is a distribution on M, then w is a distribution on $M^{\times 2}$ and, in adapted coordinates, $\partial_0 w = \partial'_0 w = 0$. The equation $K_x K_{x'} w = 0$ then reduces to an elliptic equation on $\Sigma^{\times 2}$, which implies that w is smooth (see e.g. Ref. 48, Theorem 8.3.1). $\square$

Remark 4.3. Proposition 4.2 shows in particular that there is at most one nondegenerate ground one-particle structure and at most one nondegenerate β-KMS one-particle structure at any fixed $\beta > 0$, up to unitary equivalence. These are the ones of Theorem 4.3. The degenerate ones may be classified in terms of w. In space–times with a compact Cauchy surface Σ we note that the only smooth function w with the stated properties is $w = 0$. Indeed, for any fixed $y \in \Sigma$, $v_y(x) := w(x, y)$ solves $Cv_y = 0$ for $C := -\nabla_i^{(h)}(Nh^{ij} - N^{-1}N^i N^j)\nabla_i^{(h)} + VN$. (This is because w solves the Klein–Gordon equation and is Killing time independent.) As $0 = \langle v_y, Cv_y\rangle \geq \left\|\sqrt{VN}v_y\right\|^2$ in $L^2(\Sigma)$ this implies $v_y = 0$ and hence $w = 0$.

4.2.3. *Simplifications in the standard static case*

On a standard static space–time M, the construction of the nondegenerate ground and β-KMS one-particle structures in the proof of Theorem 4.3 simplifies. For later convenience we formulate these results as a proposition:[7]

Proposition 4.3. *Let $\Sigma \subset M$ be a Cauchy surface orthogonal to the Killing field of the standard static, globally hyperbolic space–time M. Under the assumptions of Theorem 4.3 we have:*

(i) *The unique nondegenerate ground one-particle structure is given, up to equivalence, by $\mathcal{K}_0 = L^2(\Sigma)$ and $p_0 = q_{0,\Sigma} S^{-1} E$ with*

$$q_{0,\Sigma}(f_0, f_1) := \frac{1}{\sqrt{2}}\left(C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 - iC^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right).$$

Furthermore, the unitary group $\tilde{O}_t$ of Lemma 4.3 is given by $\tilde{O}_t = e^{it\sqrt{C}}$.

(ii) *For any $\beta > 0$ the unique nondegenerate β-KMS one-particle structure is given, up to equivalence, by $\mathcal{K}_{(\beta)} = L^2(\Sigma)^{\oplus 2}$ and $p_{(\beta)} = q_{(\beta),\Sigma} S^{-1} E$ with*

$$q_{(\beta),\Sigma}(f_0, f_1) := \frac{1}{\sqrt{2}}\Big(\left(I - e^{-\beta\sqrt{C}}\right)^{-\frac{1}{2}}\left(C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 - iC^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right)$$
$$\oplus\, e^{-\frac{\beta}{2}\sqrt{C}}\left(I - e^{-\beta\sqrt{C}}\right)^{-\frac{1}{2}}\left(C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 + iC^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right)\Big).$$

Furthermore, the unitary group $\tilde{O}_t$ of Lemma 4.3 is given by $\tilde{O}_t = e^{it\sqrt{C}} \oplus e^{-it\sqrt{C}}$.

Here C is the closure of the partial differential operator

$$C_0 := -\sqrt{N}\nabla^{(h),i} N \nabla^{(h)}_i \sqrt{N} + VN^2 \,,$$

defined on $C_0^\infty(\Sigma)$. C_0 and all integer powers of it are essentially self-adjoint on the invariant domain $C_0^\infty(\Sigma)$. Furthermore, C is strictly positive with $C \geq VN^2$ and $C_0^\infty(\Sigma)$ is contained in the domain of $C^{\pm\frac{1}{2}}$ for both signs.

One may also write C in terms of the conformal metric $\tilde{h}$ as

$$C = \Box_{\tilde{h}} + VN^2 + \frac{d-2}{2} N^{-2}\left(N(\Box_{\tilde{h}} N) + \frac{d-4}{2} \tilde{h}^{ij} (\partial_i N)(\partial_j N) \right),$$

on $L^2(\Sigma, d\,\mathrm{vol}_{\tilde{h}})$, where we used the footnote g on page 26 and the fact that $v = N$ in the static case. The completeness of $\tilde{h}$ (Theorem 3.2) implies that all powers of $-\Box_{\tilde{h}}$ are essentially self-adjoint on the test-functions. Proposition 4.3 shows, among other things, that the additional terms do not spoil this result.

Proof. In the standard static case $N^i \equiv 0$, so the operator A of Lemma 4.2 can be written as a diagonal matrix $A = \frac{1}{2}\begin{pmatrix} \alpha & 0 \\ 0 & N \end{pmatrix}$, where $\alpha := -\nabla^{(h),i} N \nabla^{(h)}_i + VN$. Let $\hat{\alpha}$ denote the Friedrichs extension of α, which is strictly positive by Lemmas A.7 and A.6. We may then compute $\sqrt{\hat{A}}$ and hence, on the range of $\sqrt{\hat{A}}$,

$$H_e = 2i\sqrt{\hat{A}}\sigma\sqrt{\hat{A}} = \begin{pmatrix} 0 & -i\sqrt{\hat{\alpha}}\sqrt{N} \\ i\sqrt{N}\sqrt{\hat{\alpha}} & 0 \end{pmatrix}.$$

Both $\sqrt{\hat{\alpha}}\sqrt{N}$ and $\sqrt{N}\sqrt{\hat{\alpha}}$ are closable operators, because H_e is closable. Furthermore, their closures are each others adjoints, because H_e is self-adjoint. By the Polar Decomposition Theorem (Ref. 15, Theorem 6.1.11) there is then a partial isometry U such that $\overline{\sqrt{\hat{\alpha}}\sqrt{N}} = UC^{\frac{1}{2}}$ and $\overline{\sqrt{N}\sqrt{\hat{\alpha}}} = C^{\frac{1}{2}}U^*$, where $C = \overline{\sqrt{N}\hat{\alpha}\sqrt{N}} = \overline{C_0}$. Now $H_e^2 = \begin{pmatrix} \sqrt{\hat{\alpha}}N\sqrt{\hat{\alpha}} & 0 \\ 0 & C_0 \end{pmatrix}$ on the range of $\sqrt{\hat{A}}$, which is invariant. The essential self-adjointness of all even powers of H_e on this range (Theorem 4.2), restricted to the second summand of $L^2(\Sigma)^{\oplus 2}$, implies that all integer powers of C_0 are essentially self-adjoint on the range of $\sqrt{N}$, which is just $C_0^\infty(\Sigma)$. The estimate $C \geq VN^2$ follows from a partial integration, whereas strict positivity follows from Lemma A.6. That $C_0^\infty(\Sigma)$ is in the domain of $C^{\frac{1}{2}}$ is clear, because it is in the domain of C, and that it is in the domain of $C^{-\frac{1}{2}}$ follows again from Lemma A.6. Finally, the domain and range of U are the entire $L^2(\Sigma)$, because $C^{\frac{1}{2}}$ and $\hat{\alpha}^{\frac{1}{2}}$ have dense ranges. This establishes all the claims concerning C.

Returning to one-particle structures, we may write, after some short computations:

$$V^*|H_e|V = \begin{pmatrix} C^{\frac{1}{2}} & 0 \\ 0 & C^{\frac{1}{2}} \end{pmatrix}, \quad V^*P_\pm V = \frac{1}{2}I \pm \frac{1}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},$$

$$q_{\rm cl}(f_0, f_1) = \frac{1}{\sqrt{2}} V \begin{pmatrix} C^{\frac{1}{2}} N^{-\frac{1}{2}} & 0 \\ 0 & N^{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix},$$

where we introduced the unitary operator $V := \left(\begin{smallmatrix} U & 0 \\ 0 & I \end{smallmatrix}\right)$. A comparison with the proof of Theorem 4.3 yields

$$\begin{aligned} q(f_0, f_1) = \frac{1}{2} \begin{pmatrix} U \\ iI \end{pmatrix} \left(I - e^{-\beta\sqrt{C}}\right)^{-\frac{1}{2}} \left(C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 - i C^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right) \\ \oplus \frac{1}{2} \begin{pmatrix} U \\ -iI \end{pmatrix} e^{-\frac{\beta}{2}\sqrt{C}} \left(I - e^{-\beta\sqrt{C}}\right)^{-\frac{1}{2}} \left(C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 + i C^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right), \end{aligned} \quad (4.8)$$

where we made use of the fact that $P_\pm V = \frac{1}{2}\left(\begin{smallmatrix} U \\ \mp iI \end{smallmatrix}\right)(I \pm iI)$. As $\|U\psi \oplus \pm i\psi\|^2 = \|\sqrt{2}\psi\|^2$, the first factors in each summand can safely be replaced by $\sqrt{2}$, leading to a unitary equivalent formulation, $q_{(\beta),\Sigma}$. Note that the range of $q_{(\beta),\Sigma}$ is dense in $L^2(\Sigma)^{\oplus 2}$, because if $\psi \oplus \chi$ is orthogonal to this range, then we may use the strict positivity of the operators $\left(I - e^{-\beta\sqrt{C}}\right)^{-\frac{1}{2}} C^{\pm\frac{1}{4}}$ to show that $\psi \pm e^{-\frac{\beta}{2}\sqrt{C}}\chi = 0$ for both signs and hence $\psi = \chi = 0$. The proof of the fact that $H = \sqrt{C} \oplus -\sqrt{C}$ is an easy exercise which we omit. The case of the ground one-particle structure is similar, but simpler. $\square$

The result of Proposition 4.3 can be interpreted in terms of positive and negative frequency solutions.[49] Indeed, any solution $\phi = Ef \in \mathcal{S}$ with initial data (f_0, f_1) can be decomposed into positive and negative frequency parts

$$\left(N^{-\frac{1}{2}}\phi\right)(t, \cdot) = e^{it\sqrt{C}} N^{-\frac{1}{2}} f_+ + e^{-it\sqrt{C}} N^{-\frac{1}{2}} f_-, \quad (4.9)$$

where $f_\pm = \frac{1}{2}\left(f_0 \mp i N^{\frac{1}{2}} C^{-\frac{1}{2}} N^{\frac{1}{2}} f_1\right)$. In the ground state we have

$$\omega_2^0(\bar{f}, f) = \frac{1}{2}\left\|C^{\frac{1}{4}} N^{-\frac{1}{2}} f_0 - i C^{-\frac{1}{4}} N^{\frac{1}{2}} f_1\right\|^2, \quad (4.10)$$

which vanishes when $f_0 = i N^{\frac{1}{2}} C^{-\frac{1}{2}} N^{\frac{1}{2}} f_1$, which is the case precisely when $f_+ = 0$, i.e. when ϕ is a negative frequency solution. (The occurrence of negative, rather than positive, frequency solutions here is explained by the footnote h on page 31.)

5. Ground States and their Properties

We are now ready to study the space $\mathscr{G}^0(\mathcal{W})$ of ground states, under the assumptions of Theorem 4.3, and to consider some of their properties. These properties often generalize the special properties of the Minkowski vacuum. Note that a characterization of all classical equilibrium and ground states on the commutative Weyl C^*-algebra $\mathcal{W}^{\rm cl}$ can be given, in principle, using the results of Sec. 2.

5.1. *The space of ground states*

The following theorem gives a full description of the space $\mathscr{G}^0(\mathcal{W})$ of all ground states. (This result may be compared to Theorem 2.2.)

Theorem 5.1. *Let M be a globally hyperbolic, stationary space–time and consider a linear scalar field with a stationary potential V such that $V > 0$.*

(i) *There exists a unique C^2 ground state ω^0 with vanishing one-point function. It is also the unique extremal C^1 ground state with vanishing one-point function. We denote its GNS-triple by $(\mathcal{H}_0, \pi_0, \Omega_0)$ and the one-particle structure of its two-point function is $(p_0, \mathcal{K}_0)$ (cf. Theorem 4.3).*

(ii) *ω^0 is quasi-free and regular (D^∞) and π_0 is faithful and irreducible.*

(iii) *The map $\lambda_0 := \lambda_{\omega^0}$ of Lemma 2.3 restricts to an affine homeomorphism $\lambda_0 : \mathscr{G}^0(\mathcal{W}^{\mathrm{cl}}) \to \mathscr{G}^0(\mathcal{W})$.*

(iv) *Any D^2 ground state is Hadamard and any regular ground state satisfies the microlocal spectrum condition. A ground state $\omega = \lambda_0(\rho)$ is C^k, respectively D^k, $k = 1, 2, \ldots,$ if and only if ρ is C^k, respectively D^k.*

(v) *Any extremal ground state ω on $\mathcal{W}$ is of the form $\omega = \eta_\rho^* \omega^0$ for some gauge transformation of the second kind η_ρ. Hence it is pure and it is regular (respectively C^∞) if and only if it is D^1 (respectively C^1). Furthermore, it has the Reeh–Schlieder property, i.e. for any open set $O \subset M$ the linear space $\pi_\omega(\mathcal{W}(O))\Omega_\omega$ is dense in $\mathcal{H}_\omega$.*

(vi) *If there exists an $\epsilon > 0$ such that $VN \geq \epsilon$ and $N^{-1}v^2 \geq \epsilon$ everywhere, then $(p_0, \mathcal{K}_0)$ has a mass gap,[j] namely $\|H^{-1}\| \leq \epsilon^{-1}$.*

(vii) *For $d = 4$, Haag duality holds: if $\Sigma \subset M$ is a Cauchy surface, $U \subset \Sigma$ an open, relatively compact subset whose boundary ∂U is a smooth submanifold of Σ and $O := D(U)$, then*

$$\pi_0(\mathcal{W}(O))' = \pi_0(\mathcal{W}(O^\perp))'' ,$$

where $O^\perp := \mathrm{int}(M \setminus J(O))$ denotes the causal complement for any subset $O \subset M$.

Recall that the Reeh–Schlieder property means that the ground state has many nonlocal correlations.[41,50] In fact, the Reeh–Schlieder property is known for all quasi-free D^∞ equilibrium states.[51]

Proof. Let ω^0 be the quasi-free state whose two-point distribution is associated to the nondegenerate ground one-particle structure $(p_0, \mathcal{K}_0)$ of Theorem 4.3. Then ω^0 is a nondegenerate and pure (and hence extremal) ground state, by Theorems 2.3 and 2.1. As ω^0 is quasi-free and ω^0_2 is a distribution (density), ω^0 is a regular state. Furthermore, the representation π_0 is irreducible, because ω^0 is pure, and it is

[j] Our condition is weaker than that of Ref. 7, which requires $N^{-1}v^2 \geq \epsilon$, $V \geq \epsilon$ and $N \geq \epsilon$.

faithful, because the space (L, E) is symplectic (by construction) and hence $\mathcal{W}$ is simple (Ref. 14, Theorem 5.2.8).

Using Lemma 4.3 and the fact that ω^0 is quasi-free one may show that the strong derivatives of $t \mapsto \pi_0(\alpha_t(W(f)))\Omega_0$ are well defined for all $f \in L$. The map $\lambda_0 := \lambda_{\omega^0}$ of Lemma 2.3 then restricts to the stated affine homeomorphism by Proposition 2.4.

For regular ground states, the Hadamard property is known to hold[52] and the microlocal spectrum then follows.[44,45] The Hadamard property for D^2 ground states then follows from the last statement of Proposition 4.2. From the definition of λ_0 we have

$$(\lambda_0\rho)(W(f_1)\cdots W(f_n)) = \omega^0(W(f_1)\cdots W(f_n))\rho(W(f_1)\cdots W(f_n))\,.$$

As ω^0 is regular and quasi-free it follows that $\lambda_0(\rho)$ is C^k (respectively D^k) if and only if ρ is C^k (respectively D^k).

Extremal ground states ω on $\mathcal{W}$ are of the form $\lambda_0(\rho)$ for an extremal ground state ρ on $\mathcal{W}^{\mathrm{cl}}$. Such ρ are pure by Theorem 2.2, so by Lemma 2.3 this entails $\omega = \eta_\rho^*\omega^0$. Because η_ρ^* preserves pure states it follows that every extremal ground state on $\mathcal{W}$ is pure (cf. Remark 2.2). Furthermore, η_ρ^* preserves the local algebras $\mathcal{W}(O)$, so the extremal ground states have the Reeh–Schlieder property, because ω^0 does.[51] The statement on the regularity of extremal ground states follows directly from Proposition 2.2. This also proves the second uniqueness clause for ω^0. The first uniqueness clause follows from Theorem 2.4.

To prove the existence of the mass gap we note that, under the stated assumptions, $\hat{A} \geq \frac{\epsilon}{2}I$ by Lemma 4.2. In the energetic Hilbert space we then use $(i\sigma)^* = i\sigma$ to estimate

$$H_e^2 = 4\hat{A}^{\frac{1}{2}}i\sigma\hat{A}i\sigma\hat{A}^{\frac{1}{2}} \geq 2\epsilon\hat{A}^{\frac{1}{2}}(i\sigma)^2\hat{A}^{\frac{1}{2}} = 2\epsilon\hat{A} \geq \epsilon^2 I\,.$$

Hence, $|H_e| \geq \epsilon I$, $H \geq \epsilon I$ and $\|H^{-1}\| < \epsilon^{-1}$.

Finally, the fact that ω is pure entails Haag duality, at least when $d = 4$ (Ref. 53, Theorem 3.6), even for slightly more general regions O than used here. □

A few remarks concerning the interpretation of the results of this section and their implications are in order:

Remark 5.1. The gauge transformations of the second kind, which appeared in the proof of Theorem 5.1, can be physically interpreted as field redefinitions. If ω_1 is a linear map on L, then $\chi := e^{-i\omega_1}$ is a character and $\rho(W(f)) := e^{-i\omega_1(f)}$ defines a pure state on $\mathcal{W}^{\mathrm{cl}}$. If we write (formally) $W(f) = e^{i\Phi(f)}$ we have

$$\eta_\rho(W(f)) = e^{i(\Phi(f)-\omega_1(f)I)}\,.$$

In particular, if ω is any pure C^2 ground state with one-point distribution ω_1 and ρ is defined as above, then we must have $\eta_\rho^*\omega = \omega^0$ by Theorem 5.1. Hence, $\omega(W(f)) = e^{i\omega_1(f)}\omega^0(W(f))$. Because pure states ρ of this exponential form are dense (Ref. 19, Lemma 4.2) we may argue on physical grounds that we may as well restrict attention to the pure ground state with vanishing one-point distribution, ω^0.

Remark 5.2. Because ω^0 is a uniquely distinguished ground state and π_0 is faithful we may perform the following standard modification of the original theory. For each bounded region $O \subset M$ we define the von Neumann algebra $\mathcal{R}(O) := \pi_0(\mathcal{W}(O))''$. This gives rise to a local net of von Neumann algebras in the space–time M and we let the C^*-algebra $\mathcal{R}$ be their inductive limit. Each $\mathcal{R}(O)$ contains the corresponding $\mathcal{W}(O)$, so that $\mathcal{R} \supset \mathcal{W}$. We may then consider the class of states on $\mathcal{R}$ which are locally normal, i.e. they restrict to normal states on each von Neumann algebra $\mathcal{R}(O)$. Such states clearly restrict to a state on $\mathcal{W}$ and a state ω on $\mathcal{W}$ has at most one extension to $\mathcal{R}$. This extension exists if and only if ω is locally normal with respect to ω^0 (by definition). This includes at least all quasi-free Hadamard states.[54]

There are good physical reasons to consider only states on $\mathcal{W}$ that are locally normal with respect to ω^0. For any self-adjoint operator $A \in \mathcal{W}(O)$ for any bounded region O, the algebra $\mathcal{R}(O)$ contains all the spectral projectors of A, so the operational question whether the measured value of A attains a value in some Borel set $I \subset \mathbb{R}$ corresponds to the same projection operator for all locally normal states. Another reason to restrict only to locally normal states is of a more technical nature. The action of the one-parameter group α_t on $\mathcal{W}$ is not norm continuous, but the larger algebra $\mathcal{R}$ contains a C^*-algebra $\mathcal{R}_0$ which is dense in $\mathcal{R}$ in the strong operator topology and on which α_t is norm continuous (cf. Ref. 55, Sec. 4 or also Ref. 20, Theorem 1.18 for a closely related result). This means that a large number of results on C^*-dynamical systems can be brought to bear on $(\mathcal{R}_0, \alpha_t)$, and hence indirectly also on $\mathcal{W}$, if one considers states that are locally normal[14,20] with respect to ω^0.

Let us briefly describe the constructions of Ref. 55 (adapted to a stationary, globally hyperbolic space–time and with a possibly noncompact Cauchy surface). The C^*-algebra $\mathcal{R}_0$ may be generated by operators of the form

$$A_f := \int dt\, f(t)\alpha_t(A)\,,$$

where $A \in \mathcal{W}(O)$ for some bounded region O and $f \in C_0^\infty(\mathbb{R})$. Then $A_f \in \mathcal{R}(O')$, where O' is another bounded region that depends on O and on the support of f. Such operators form a *-algebra which is invariant under the action of α_t and on which α_t is norm continuous. $\mathcal{R}_0$ is the norm closure of this *-algebra.

5.2. *The ground state representation and the quantum stress-energy–momentum tensor*

As ω^0 is quasi-free, $\mathcal{H}_0$ is a Fock space (cf. Subsec. 3.2 of Ref. 8) and we may introduce a particle interpretation for the field, based on creation and annihilation operators. Note that such an interpretation fails in general space–times, because there are many unitarily inequivalent Fock space representations and there is no generally covariant prescription to single out a preferred one.[3,56]

Following standard notations[14] we will write $\mathcal{H}_0 = \bigoplus_{n=0}^{\infty} \mathcal{H}_0^{(n)}$, where the n-particle Hilbert space is $\mathcal{H}_0^{(n)} := P_+(\mathcal{K}_0)^{\otimes n}$, in which $(p_0, \mathcal{K}_0)$ is the one-particle structure associated to ω_2^0 and P_+ denotes the projection onto the symmetric tensor product. We write N for the number operator, so that $N|_{\mathcal{H}_0^{(n)}} = nI$. We will use the notation $a^*(\psi)$ and $a(\psi)$ for creation and annihilation operators, respectively, where $\psi \in \mathcal{K}_0$. As $a^*(\psi)^* = a(\psi)$ we see that a is complex antilinear in ψ, whereas a^* is linear. The field Φ is given by

$$\Phi(f) = \frac{1}{\sqrt{2}}(a^*(p_0(f)) + a(p_0(\bar{f})))$$

and is complex linear, as desired. We may introduce the initial value and normal derivative of the quantum field as

$$\Phi_0(f_1) := \frac{-1}{\sqrt{2}}(a^*(q_0(0, f_1)) + a(q_0(0, \overline{f_1}))),$$
$$\Phi_1(f_0) := \frac{1}{\sqrt{2}}(a^*(q_0(f_0, 0)) + a(q_0(\overline{f_0}, 0)))$$

so that $\Phi(f) = \Phi_1(f_0) - \Phi_0(f_1)$, where $(f_0, f_1) = S^{-1}Ef$. This is in line with what one would get if Φ were a classical solution to the Klein–Gordon equation (cf. Eq. (4.3)). It will also be convenient to introduce the operators

$$\Pi(f) := \frac{i}{\sqrt{2}}(a^*(p_0(f)) - a(p_0(\bar{f}))).$$

Because the classical stress-energy–momentum tensor played a significant role in the classical and quantum descriptions of the linear scalar field in a stationary space–time, it seems fitting to also spend a few words on the quantum stress-energy–momentum tensor. If the field theory on M can be extended to all globally hyperbolic space–times in a locally covariant way,[4] e.g. if $V = cR + m^2$, then there is a generally covariant way to define the renormalized stress-energy–momentum tensor.[57] However, in our setting it will be advantageous not to renormalize the stress tensor in a generally covariant way, but instead to exploit the extra structure of the stationary space–time. (Nevertheless, our presentation of the classical and quantum stress tensor is based on existing treatments that fit in a generally covariant framework, e.g. Ref. 58.)

We may define a tensor field G_{ab} on a sufficiently small neighborhood $U \subset M^{\times 2}$ of the diagonal $\Delta := \{(x, x) \mid x \in M\}$ by the property that for any vector $v^b \in T_{x'}M$, the vector $g^{ac}(x)G_{cb}(x, x')v^b(x') \in T_xM$ is the parallel transport of v along a unique geodesic connecting x to x'. (The uniqueness of the geodesic can be ensured by choosing U sufficiently small.) Using G_{ab} and $G^{ab}(x, x') := g^{ac}(x)g^{bd}(x')G_{cd}(x, x')$ we may write the classical stress-energy–momentum tensor in terms of a differential operator as

$$\begin{aligned} T_{ab}(\phi) &= \left(T_{ab}^{\mathrm{split}}\phi^{\otimes 2}\right)(x,x)\,,\\ T_{ab}^{\mathrm{split}} &= \nabla_a\otimes\nabla_b - \frac{1}{2}G_{ab}G^{cd}\nabla_c\otimes\nabla_d - \frac{1}{2}G_{ab}\sqrt{V}\otimes\sqrt{V}\,. \end{aligned} \tag{5.1}$$

Instead of letting the operator T_{ab}^{split} act on the classical fields $\phi^{\otimes 2}$, we can let it act on the normal ordered quantum field,

$$:\Phi^{\otimes 2}:(x,x') = \Phi(x)\Phi(x') - \omega_2^0(x,x')\,.$$

For any vector $\psi\in\pi_0(\mathcal{A})\Omega_0$ we may define the $\mathcal{H}_0$-valued distribution (density)

$$T_{ab}^{\mathrm{ren}}(f^{ab})\psi := \lim_{n\to\infty} T_{ab}^{\mathrm{split}}:\Phi^{\otimes 2}:(f^{ab}\delta_n)\psi\,,$$

where $\delta_n\in C^\infty(M^{\times 2})$ is a sequence of functions that approximates the delta distribution $\delta(x,x')$ and f^{ab} is a compactly supported, smooth test-tensor.[45] The operator $T_{ab}^{\mathrm{ren}}(f^{ab})$ is densely defined and it is a symmetric operator when f^{ab} is real-valued. Moreover, if $V>0$ everywhere one can show that $T_{ab}^{\mathrm{ren}}(\chi^a\chi^b)$ is semi-bounded from below for real-valued test-vector fields χ^a.[58] (Note that the method of proof in Ref. 58 is not affected by the presence of the nonnegative potential energy term V in the equation of motion.)

In analogy with the classical case we define the quantum energy–momentum one-form and the energy density by

$$P_a^{\mathrm{ren}}(f^a) := T_{ab}^{\mathrm{ren}}(f^a\xi^b)\,,\quad \epsilon^{\mathrm{ren}}(f) := T_{ab}^{\mathrm{ren}}(n^a\xi^b f)$$

in the sense of $\mathcal{H}_0$-valued distributions, when acting on $\pi_0(\mathcal{A})\Omega_0$. One may check that T_{ab}^{ren} is symmetric in its indices a,b and that

$$\nabla^a T_{ab}^{\mathrm{ren}} = -(\nabla_b V):\Phi^2:\,,$$

where the Wick square $:\Phi^2:$ is the restriction of $:\Phi^{\otimes 2}:$ to the diagonal $\Delta\subset M^{\times 2}$. It follows from $\partial_0 V=0$ that $\nabla^a P_a^{\mathrm{ren}}=0$, just like in the classical case.

Remark 5.3. From a physical point of view it seems reasonable to expect that for real-valued f the operator $\epsilon^{\mathrm{ren}}(f^2)$ is semi-bounded from below, using the same motivation as for existing quantum inequalities.[58] However, the details of the argument require that we can write $\xi^a n^b + n^a\xi^b = \sum_{j=1}^k \chi_j^a\chi_j^b$ for some finite number of (real) vectors χ_j^a. An easy exercise shows that this is possible if and only if we are in the static case, where $\xi^a = Nn^a$, in which case the single vector $\chi^a = N^{-\frac{1}{2}}\xi^a$ will suffice. Thus, in the static case, the results of Ref. 58 apply and $\epsilon^{\mathrm{ren}}(f^2)$ is semi-bounded from below.

There is another result, however, which does work very nicely in the general stationary setting:

Theorem 5.2. *Under the assumptions of Theorem* 5.1, *let* ω^0 *be the unique ground state. For any real-valued test-tensor* f^{ab}, *the operator* $T_{ab}^{\mathrm{ren}}(f^{ab})$ *is essentially self-adjoint on* $\pi_0(\mathcal{A})\Omega_0$.

A similar essential self-adjointness result for the smeared stress-energy–momentum tensor in general globally hyperbolic space–times is much harder to obtain by a direct proof (cf. Ref. 59 for partial results).

Proof. It follows from Lemma 4.3 (and second quantization) that the Hamiltonian operator h is essentially self-adjoint on the dense, invariant domain $\pi_0(\mathcal{A})\Omega_0$ and that

$$\langle\psi,[h+I,T^{\mathrm{ren}}_{ab}(f^{ab})]\psi'\rangle=\langle\psi,iT^{\mathrm{ren}}_{ab}(\partial_0 f^{ab})\psi'\rangle\,,$$

for all ψ, ψ' in that domain. (Here we have used the fact that ω^0 is an equilibrium state.) The idea is now to use the Commutator Theorem X.36' of Ref. 21 to prove essential self-adjointness of $T^{\mathrm{ren}}_{ab}(f^{ab})$. This means we need to prove that for any test-tensor f^{ab} there is a $C>0$ such that

$$|\langle\psi,T^{\mathrm{ren}}_{ab}(f^{ab})\psi'\rangle|\le C\big\|(h+I)^{\frac{1}{2}}\psi\big\|\cdot\big\|(h+I)^{\frac{1}{2}}\psi'\big\|\,, \tag{5.2}$$

for all ψ, $\psi'\in\pi_0(\mathcal{A})\Omega_0$. By polarization it suffices to take $\psi=\psi'$. It also suffices to consider f^{ab} to be supported in a convex normal neighborhood, by a partition of unity argument. Moreover, the antisymmetric part of f^{ab} does not contribute and the symmetric part can be written as a finite sum of terms of the form $\chi^a\chi^b$, so it suffices to consider $f^{ab}=\chi^a\chi^b$.

Now consider the operators $\Pi(f)$ for $f\in C_0^\infty(M)$. $[\Pi(f),\Pi(f')]=[\Phi(f),\Phi(f')]=iE(f,f')$, so for any $\psi\in\pi_0(\mathcal{A})\Omega_0$ the distribution

$$\omega_2^\psi(f,f'):=\|\psi\|^{-2}\langle\psi,\Pi(f)\Pi(f')\psi\rangle$$

is a Hadamard two-point distribution. As for the field $\Phi(f)$ one may introduce the normal-ordered product $:\Pi(f)\Pi(f'):\,:=\Pi(f)\Pi(f')-\omega_2^0(f,f')$ and following Ref. 58 one proves that the operator

$$\tilde{T}^{\mathrm{ren}}_{ab}(\chi^a\chi^b):=\big(T^{\mathrm{split}}_{ab}:\Pi^{\otimes 2}:\big)(\chi^a\chi^b\delta)$$

is semi-bounded from below. Hence, for some $c>0$,

$$T^{\mathrm{ren}}_{ab}(\chi^a\chi^b)\le T^{\mathrm{ren}}_{ab}(\chi^a\chi^b)+\tilde{T}^{\mathrm{ren}}_{ab}(\chi^a\chi^b)+cI=2\big(T^{\mathrm{split}}_{ab}a^*\otimes a\big)(\chi^a\chi^b\delta)+cI\,. \tag{5.3}$$

The first term on the right-hand side is the second quantization of an operator T on $\mathcal{H}_0^{(1)}$, for which we have

$$\begin{aligned}\langle\Phi(f)\Omega_0,T\Phi(f)\Omega_0\rangle&=2\big(T^{\mathrm{split}}_{ab}\bar{\phi}\otimes\phi\big)(\chi^a\chi^b\delta)\\&=\int_M|\chi^a\nabla_a\phi|^2-\chi^a\chi_a g^{bc}\,\overline{\nabla_b\phi}\,\nabla_c\phi-\chi^a\chi_a V|\phi|^2\\&\le c'\int_{\mathrm{supp}(\chi^a)}|\partial_0\phi|^2+h^{ij}\,\overline{\nabla^{(h)}_i\phi}\,\nabla^{(h)}_j\phi+|\phi|^2\,,\end{aligned} \tag{5.4}$$

for some $c' > 0$, where we defined $\phi := \omega_2^0(\cdot\,, f)$. On the other hand, because the classical energy is independent of the Cauchy surface, h satisfies (cf. Lemma 4.2)

$$\begin{aligned}\mathcal{E}(\phi) &= \langle \Phi(f)\Omega_0, h\Phi(f)\Omega_0\rangle \\ &= \int_M \frac{\tau(t)}{2N^2}\Big(|\partial_0\phi|^2 + (N^2h^{ij} - N^iN^j)\overline{\nabla_i^{(h)}\phi}\nabla_j^{(h)}\phi + VN^2|\phi|^2\Big)\,, \quad (5.5)\end{aligned}$$

where $\tau \in C_0^\infty(\mathbb{R})$ satisfies $\int \tau = 1$. Choosing $\tau \geq 0$ and $\tau > 0$ on the compact support of χ^a and using the fact that $Nh^{ij} - N^{-1}N^iN^j$ is positive definite, the desired estimate Eq. (5.2) easily follows from Eqs. (5.3)–(5.5). $\square$

Note that $\big[T_{ab}^{\mathrm{ren}}(f^{ab}), \pi_0(W(f'))\big] = 0$ whenever $\mathrm{supp}(f') \cap J(\mathrm{supp}(f^{ab})) = \emptyset$. It follows from Haag duality that $T_{ab}^{\mathrm{ren}}(f^{ab})$ is affiliated to the local von Neumann algebra $\mathcal{R}(D(\mathrm{supp}(f^{ab})))$.

Lemma 5.1. *Let Σ be Cauchy surface in a stationary, globally hyperbolic space–time M. Let $f \in C_0^\infty(M)$, $\tau \in C_0^\infty(\mathbb{R})$ with $\int \tau = 1$ and $\chi \in C_0^\infty(\Sigma)$ such that $\chi \equiv 1$ on $\mathrm{supp}(\tau) \cap J(\mathrm{supp}(f))$, where we view τ, χ as functions on M in adapted coordinates. Then*

$$\big[\epsilon^{\mathrm{ren}}(\tau \otimes N^{-1}\chi), \Phi(f)\big] = \Phi(i\partial_0 f)$$

on $\pi_0(\mathcal{A})\Omega_0$.

Proof. We follow the computations in Ref. 55, App. A.2. Fix a vector $\psi \in \pi_0(\mathcal{A})\Omega_0$, so that $\phi' := \langle \psi, \Phi(\cdot)\psi\rangle$ is a smooth function. Let $\phi := E(\cdot\,, f)$ and note that $\partial_0\phi = E(\cdot\,, \partial_0 f)$, by the uniqueness of $E^\pm$. Using $\omega\big(\big[:\Phi^{\otimes 2}:(x,x'), \Phi(f)\big]\big) = i\phi(x)\phi'(x') + i\phi'(x)\phi(x')$ we find after some algebra

$$\omega([\epsilon^{\mathrm{ren}}(\cdot), \Phi(f)]) = i(Nh^{ij} - N^{-1}N^iN^j)\partial_i\phi\partial_j\phi' + iVN\phi\phi' + iN^{-1}\partial_0\phi\partial_0\phi'\,.$$

Using the Klein–Gordon equation and Eq. (4.3) we may then compute for any Cauchy surface Σ'

$$\begin{aligned}\omega(\Phi(i\partial_0 f)) &= i\int_M (\partial_0 f)\phi' = -i\int_{\Sigma'} (n^a\nabla_a\partial_0\phi)\phi' - (\partial_0\phi)n^a\nabla_a\phi' \\ &= i\int_{\Sigma'} (Nh^{ij} - N^{-1}N^iN^j)\partial_i\phi\partial_j\phi' + VN\phi\phi' + N^{-1}\partial_0\phi\partial_0\phi' \\ &= \int_{\Sigma'} \omega([\epsilon^{\mathrm{ren}}(\cdot), \Phi(f)]) = \int_M \tau(t)N^{-1}\chi\omega([\epsilon^{\mathrm{ren}}(\cdot), \Phi(f)])\,.\end{aligned}$$

By polarization the desired operator equality now holds on the indicated dense domain. $\square$

6. KMS States in Stationary Space–Times

We now come to the thermal equilibrium states at nonzero temperature. We still consider a linear scalar field in a stationary, globally hyperbolic space–time and we assume that the theory has a unique C^2 ground state ω^0 as in Sec. 5 and a Hamiltonian operator h. In Subsec. 6.2, we will review the states satisfying the KMS-condition, which exist for every inverse temperature $\beta > 0$. Afterwards, in Subsec. 6.3, we show that their two-point distributions can be obtained from a Wick rotation, in case M is standard static (see also Ref. 5).

Before we come to this, however, we study the motivation to use the KMS-condition as a characterization of thermal equilibrium in Subsec. 6.1. In particular we show that for a standard static space–time M with compact Cauchy surfaces we may also define Gibbs states to describe thermal equilibrium and these Gibbs states satisfy the KMS-condition.

6.1. *Gibbs states and the KMS-condition*

Consider, then, a stationary, globally hyperbolic space–time M and a linear scalar field satisfying the assumptions of Theorem 5.1. If, for some inverse temperature $\beta > 0$, the operator $e^{-\beta h}$ is of trace-class in the ground state representation π_0, i.e. if it has a finite trace, one may define the thermal equilibrium state to be the Gibbs state

$$\omega^{(\beta)}(A) := \frac{\mathrm{Tr}(e^{-\beta h}A)}{\mathrm{Tr}\, e^{-\beta h}}\,. \tag{6.1}$$

Here we use the fact that the set of bounded trace-class operators on a Hilbert space forms a *-ideal in the algebra of all bounded operators (Ref. 15, Remark 8.5.6 or Ref. 21, Theorem VI.19).

We now show that these Gibbs states are well defined whenever M is standard static and has compact Cauchy surfaces. Moreover, we explain that these Gibbs states satisfy the KMS-condition.

Theorem 6.1. *We make the assumptions of Theorem* 5.1 *with the additional assumptions that M is a standard static space–time with compact Cauchy surfaces, so that the theory has a mass gap. For any $\beta > 0$*

(i) $e^{-\beta h}$ *is of trace-class and in particular the Gibbs state $\omega^{(\beta)}$ of Eq.* (6.1) *is well defined and normal with respect to the ground state ω^0;*
(ii) *the Gibbs state $\omega^{(\beta)}$ is quasi-free and satisfies the KMS-condition at inverse temperature $\beta > 0$.*

Proof. By Ref. 14, Proposition 5.2.27, the operator $e^{-\beta h}$ has a finite trace on $\mathcal{H}_0$ if and only if $e^{-\beta H}$ has a finite trace on $\mathcal{H}_0^{(1)} \simeq \mathcal{K}$ and βH is strictly positive. The latter is satisfied by our assumptions, so we only need to show that $e^{-\beta H}$ has a finite trace. Our proof of this fact is adapted from the proof of nuclearity in Ref. 60.

We refer to Proposition 4.3 for a convenient formulation of the ground one-particle structure, with $\mathcal{K} \simeq L^2(\Sigma)$ and $H = \sqrt{C}$. By assumption, the theory has a mass gap, so $\sqrt{C} \geq \epsilon I > 0$. The exponential $e^{-\beta\sqrt{C}}$ is bounded and may be written as $C^{-n}(C^n e^{-\beta\sqrt{C}})$ for any $n \geq 1$, where both C^{-n} and the product in brackets are bounded. Because trace-class operators form an ideal in the algebra of bounded operators, it suffices to prove that C^{-n} is trace-class. The operator C is a partial differential operator, while C^{-2n} defines a distribution density u on $\Sigma^{\times 2}$ by Theorem A.1. We then have $(C^n u C^n)(x,y) = \delta(x,y)$. Note that $C \otimes C$ is an elliptic operator on $\Sigma^{\times 2}$. Choosing n large enough, we can make u continuous. Because Σ is compact it follows that $u \in L^2(\Sigma^{\times 2})$, which implies that it is Hilbert–Schmidt (Ref. 21, Theorem VI.23) and, by definition of Hilbert–Schmidt operators, C^{-n} is trace-class. $\omega^{(\beta)}$ is normal with respect to the ground state by definition. This completes the proof of the first item.

The quasi-free property follows from Proposition 5.2.28 of Ref. 14. For the KMS-condition we follow Ref. 12 and note that the function

$$f(z) := \pi_0(A)e^{izh}\pi_0(B)e^{-izh}e^{-\beta h} = \pi_0(A)e^{-\tau h}e^{ith}\pi_0(B)e^{-ith}e^{(\tau-\beta)h}$$

takes values in the bounded operators on $\mathcal{H}_0$ for $z = t + i\tau \in \overline{\mathrm{S}_\beta}$, as $0 \leq \tau \leq \beta$. By Lemma A.8 it is continuous on $\overline{\mathrm{S}_\beta}$ and holomorphic on the interior S_β. Moreover, $f(z)$ is trace-class, because either $e^{(\tau-\beta)h}$ or $e^{-\tau h}$ is trace-class. Using the fact that $|\operatorname{Tr}(CD)| \leq \|C\| \operatorname{Tr}|D|$ for all bounded operators C and trace-class operators D,[k] we see that $\operatorname{Tr} f(z)$ is a bounded, continuous function on $\overline{\mathrm{S}_\beta}$, which is holomorphic in the interior. Dividing by $\operatorname{Tr} e^{-\beta h}$ proves the second item. □

We see that, under suitable physical (and technical) conditions, Gibbs states are well defined for systems in a finite spatial volume. In fact, we will see in Theorem 6.2 below that for given $\beta > 0$ it is the only β-KMS state on $\mathcal{W}$ satisfying some natural additional conditions. In general, however, the given exponential operator is not of trace-class and the definition of the Gibbs state does not make sense. In such cases one takes the KMS-condition to be the defining property of thermal equilibrium states. Theorem 6.1, together with the uniqueness result of Theorem 6.2 below, is a good indication that such a definition is justified. Further evidence comes from the analysis of Ref. 13, who investigated the second law of thermodynamics for general C^*-dynamical systems. They call a state ω of such a system completely passive, if it is impossible to extract any work from any finite set of identical copies of this system, all in the same state, by a cyclic process. They then showed, among other things, that a state is completely passive if and only if it is a ground state or a KMS

[k] Proof: If D is trace-class, we may choose an orthonormal eigenbasis ψ_n of $|D|$ and use the Polar Decomposition Theorem (Ref. 15, Theorem 6.1.11) to write $D = U|D|$ for some partial isometry U. Then,

$$|\operatorname{Tr}(CD)| = \Big|\sum_n \langle U^*C^*\psi_n, |D|\psi_n\rangle\Big| \leq \|U^*C^*\| \sum_n \| |D|\psi_n\| = \|C\| \operatorname{Tr}|D| \,.$$

state at an inverse temperature $\beta \geq 0$.[l] This analysis applies to our situation, if we restrict attention to states which are locally normal with respect to the ground state (cf. Remark 5.2). We will see in Subsec. 6.2 that quasi-free, D^2 KMS states do indeed satisfy this local normality condition, because they are Hadamard. A more general and detailed study of the relations between passivity, the Hadamard condition and quantum energy inequalities was made by Ref. 55.

Probably the most direct motivation in favor of the KMS-condition is an analysis of Ref. 12 (see also Ref. 14) which shows, in the context of quantum statistical mechanics, that a thermodynamic (infinite volume) limit of Gibbs states satisfies the KMS-condition. Reformulated to our geometric setting, the idea is to approximate h by operators h_O, where $O \subset \Sigma$ has finite volume, such that $e^{ith_O} \in \mathcal{R}(D(O)) = \pi_0(\mathcal{W}(D(O)))''$ for all $t \in \mathbb{R}$, where $D(O) \subset M$ denotes the domain of dependence. If $e^{-\beta h_O}$ is a trace-class operator on $\mathcal{H}_0(O) := \overline{\pi_0(\mathcal{W}(D(O)))\Omega_0}$ for some $\beta > 0$, then it gives rise to a Gibbs state $\omega^{(\beta,O)}$. The argument of Ref. 12 shows that, under some additional assumptions on the h_O, one may show that the thermodynamic limit $\omega^{(\beta)} := \lim_{O\to\Sigma} \omega^{(\beta,O)}$ exists and is a β-KMS state. In the case of nonrelativistic point-particles in Minkowski space–time, an explicit construction of the approximate Hamiltonians h_O and the corresponding limiting procedure is described in detail in Ref. 14 (see also the classic paper Ref. 61, where the thermodynamic limit of a nonrelativistic free Bose gas was investigated in detail).

For a quantum field it is tempting to choose h_O to be of the form $h_O = \epsilon^{\mathrm{ren}}(f)$ for some suitable $f \in C_0^\infty(D(O))$, in view of Theorem 5.2 and Lemma 5.1. However, the argument becomes more problematic for two reasons. First, the restriction to a bounded open region O does not entail the desired reduction in the degrees of freedom, due to the Reeh-Schlieder property: if O is nonempty, the subalgebra $\mathcal{R}(D(O))$ already generates the entire Hilbert space $\mathcal{H}_0$ when acting on the ground state vector Ω_0. Second, and more to the point, the operators $e^{-\beta h_O}$ cannot be trace-class. In fact, $\mathcal{R}(D(O))$ is a type III_1 factor (Theorem 3.6(g)) of Ref. 53), so the only trace-class operator $X \in \mathcal{R}(D(O))$ is $X = 0$.[m] This means that no h_O can possibly satisfy the assumptions made in Ref. 12. Even in a space–time with a compact Cauchy surface Σ, the Reeh–Schlieder property of the ground state and the type of the local von Neumann algebras prevent us from finding appropriate Gibbs states to define thermal equilibrium states in any bounded region $V \subset \Sigma$

[l] If it is impossible to extract any work from only one copy of this system in the given state, the state is called passive. The set of passive states also contains convex combinations of the ground and KMS states.

[m] For a proof, consider a trace-class operator $X \in \mathcal{R}(D(O))$, so that $|X|$ has a discrete spectrum. Suppose that $P \in \mathcal{R}(D(O))$ is a spectral projection operator onto an eigenspace with an eigenvalue $c \neq 0$. As $|X|$ is trace-class, P must project onto a finite-dimensional subspace, so it is a finite projection in the von Neumann algebra $\mathcal{R}(D(O))$. However, since $\mathcal{R}(D(O))$ is a type III_1 factor, it does not have any nontrivial finite projections.[15] Thus, $P = 0$ and the only possible eigenvalue of $|X|$ is 0, which entails $X = 0$.

which is strictly smaller than Σ. All this in spite of naive physical intuition and the positive results for quantum statistical mechanics.

It is possible that other techniques, such as local entropy arguments,[62] can be employed to elucidate the local aspects of thermal equilibrium for quantum fields, but we are not aware of a detailed treatment of this issue. We must therefore conclude that, even though it is still perfectly satisfactory to use the KMS-condition as the defining property of global thermal equilibrium, the local aspects of thermal equilibrium and temperature of a quantum field are presently not well understood.

6.2. *The space of KMS states*

We now give a full description of the space $\mathscr{G}^{(\beta)}(\mathcal{W})$ of all β-KMS states in general stationary, globally hyperbolic space–times. (This result may be compared to Theorems 2.2 and 5.1.)

Theorem 6.2. *Let M be a globally hyperbolic, stationary space–time and consider a linear scalar field with a stationary potential V such that $V > 0$. Let $\beta > 0$.*

(i) *There exists a unique extremal C^1 β-KMS state $\omega^{(\beta)}$ with vanishing one-point function. We denote its GNS-triple by $\left(\mathcal{H}_{(\beta)}, \pi_{(\beta)}, \Omega_{(\beta)}\right)$ and we let h be the self-adjoint generator of the unitary group that implements α_t in this GNS-representation. The one-particle structure of its two-point function is $\left(p_{(\beta)}, \mathcal{K}_{(\beta)}\right)$ (cf. Theorem 4.3).*
(ii) *$\omega^{(\beta)}$ is quasi-free, regular (D^∞), locally quasi-equivalent to ω^0 and $\pi_{(\beta)}$ is faithful.*
(iii) *The map $\lambda_{(\beta)} := \lambda_{\omega^{(\beta)}}$ of Lemma 2.3 restricts to an affine homeomorphism $\lambda_{(\beta)} : \mathscr{G}^0(\mathcal{W}^{\mathrm{cl}}) \to \mathscr{G}^{(\beta)}(\mathcal{W})$.*
(iv) *Any D^2 β-KMS state is Hadamard and any regular β-KMS state satisfies the microlocal spectrum condition. A β-KMS state $\omega = \lambda_{(\beta)}(\rho)$ is C^k, respectively D^k, $k = 1, 2, \ldots$, if and only if ρ is C^k, respectively D^k.*
(v) *Any extremal β-KMS state ω on $\mathcal{W}$ is of the form $\omega = \eta_\rho^* \omega^0$ for some gauge transformation of the second kind η_ρ. It is regular (respectively C^∞) if and only if it is D^1 (respectively C^1). Furthermore, it has the Reeh–Schlieder property.*
(vi) *$\lim_{\beta\to\infty} \omega^{(\beta)} = \omega^0$ in the weak*-topology.*
(vii) *$\pi_\omega(\mathcal{W}) \in D(e^{-\frac{\beta}{2}h})$ and for all A, $B \in \mathcal{W}$*

$$\langle \pi_\omega(A^*)\Omega_\omega, \pi_\omega(B^*)\Omega_\omega \rangle = \left\langle e^{-\frac{\beta}{2}h}\pi_\omega(B)\Omega_\omega, e^{-\frac{\beta}{2}h}\pi_\omega(A)\Omega_\omega \right\rangle.$$

Proof. Let $\omega^{(\beta)}$ be the quasi-free state whose two-point distribution is associated to the nondegenerate β-KMS one-particle structure $(p_{(\beta)}, \mathcal{K}_{(\beta)})$ of Theorem 4.3. Then $\omega^{(\beta)}$ is a β-KMS state, by Theorem 2.3. As $\omega^{(\beta)}$ is quasi-free and $\omega_2^{(\beta)}$ is a distribution (density), $\omega^{(\beta)}$ is a regular state. The representation $\pi_{(\beta)}$ is faithful, as in the proof of Theorem 5.1.

The map $\lambda_{(\beta)} := \lambda_{\omega^{(\beta)}}$ of Lemma 2.3 restricts to the stated affine homeomorphism by Proposition 2.4. For regular β-KMS states the Hadamard property is known to hold[52] and the microlocal spectrum then follows.[44,45] The Hadamard property for D^2 β-KMS states then follows from the last statement of Proposition 4.2. The fact that $\lambda_{(\beta)}(\rho)$ is C^k (respectively D^k) if and only if ρ is, is shown as in Theorem 5.1.

Local quasi-equivalence of all quasi-free Hadamard states was proved in Ref. 54, which applies in particular to $\omega^{(\beta)}$ and ω^0.

Extremal β-KMS states ω on $\mathcal{W}$ are of the form $\omega = \eta_\rho^* \omega^0$, as in Theorem 5.1, and the Reeh–Schlieder property for ω follows from that of $\omega^{(\beta)}$.[51] The statement on the regularity of extremal β-KMS states follows directly from Proposition 2.2. This also proves the uniqueness clause for $\omega^{(\beta)}$.

Using Theorem 4.3 one may show that $\lim_{\beta\to\infty} \omega_2^{(\beta)}(f,f) = \omega_2^0(f,f)$. Indeed, the range of p_{cl} is in the domain of $|H_e|^{-1}$ by Proposition 4.2 and the functions $F(x) := e^{-\frac{\beta}{2}x}\sqrt{\frac{x}{1-e^{-\beta x}}}$ and $G(x) := \sqrt{\frac{x}{1-e^{-\beta x}}} - \sqrt{x}$ converge uniformly to 0 on the positive half line as $\beta \to \infty$. The explicit expression for $p_{(\beta)}$ and the Spectral Calculus Theorem for the functions $F(|H_e|)$ and $G(|H_e|)$ then prove the claim. It follows that $\lim_{\beta\to\infty} \omega^{(\beta)}(W(f)) = \omega^0(W(f))$, because the $\omega^{(\beta)}$ and ω^0 are quasi-free. Hence, $\lim_{\beta\to\infty} \omega^{(\beta)} = \omega^0$.

As $\omega^{(\beta)}$ is locally normal with respect to ω^0, it extends in a unique way to a locally normal state on $\mathcal{R}$, which contains a dense, C^*-dynamical system $\mathcal{R}_0$ (cf. Remark 5.2), for which ω is again a β-KMS state (by Proposition 2.1 and a limit argument). The GNS-representation π_ω of ω on $\mathcal{R}$ restricts to the GNS-representations of $\mathcal{R}_0$ and of $\mathcal{W}$, which all generate the same Hilbert space $\mathcal{H}_\omega$. The final item then follows from Ref. 20, Theorem 4.3.9. □

It is known that the state $\omega^{(\beta)}$ is not pure, but it can be purified by extending it to a so-called doubled system.[63] This abstract procedure finds a natural interpretation in the setting of black hole thermodynamics.[38] Because $\omega^{(\beta)}$ is not pure we cannot use Theorem 2.4 to obtain a uniqueness result, unlike the ground state case.

6.3. *Wick rotation in static space–times*

In Subsec. 4.2, we have shown the existence of unique nondegenerate β-KMS one-particle structures for a linear scalar quantum field on a stationary, globally hyperbolic space–time, provided the interaction potential is stationary and everywhere strictly positive. In this section, we will show that the corresponding two-point distributions can also be obtained by a Wick rotation, in case the space–time is standard static. The geometric backbone of the argument was already presented in Subsec. 3.3, so in this section we may focus on the functional analytic aspects of the technique of Wick rotation. The results we describe correspond to those in Ref. 5, but our presentation focusses more on the operator theoretic language. The case of $R = \infty$, which leads to a ground state, has already been described in some detail,[49] so we will focus primarily on the case $R < \infty$.

6.3.1. *The Euclidean Green's function*

For some $R > 0$ consider the complexification M_R^c and the associated Riemannian manifold M_R of a standard static globally hyperbolic space–time M. Because the Laplace–Beltrami operator $\Box$ on M is defined in terms of the metric and the potential V is assumed stationary, there is a natural corresponding Euclidean Klein–Gordon operator on M_R, namely $K_R := -\Box_{g_R} + V$. Our first task is to find a preferred Euclidean Green's function, which will be the starting point for the Wick rotation that should lead to a two-point distribution on the Lorentzian space–time M.

Definition 6.1. A *Euclidean Green's function* is a distribution (density) G_R on $M_R^{\times 2}$ which is a fundamental solution, $(K_R)_x G_R(x,y) = (K_R)_y G_R(x,y) = \delta(x,y)$, of positive type, $G_R(\bar{f}, f) \geq 0$ for all $f \in C_0^\infty(M_R)$.

Just like there are many (Hadamard) two-point distributions on M, there may be many Green's functions on M_R. The common wisdom is to obtain a preferred one by the following method: the partial differential operator K_R can be viewed as a positive, symmetric linear operator on the domain $C_0^\infty(M_R)$ in $L^2(M_R)$. Assuming $\overline{K_R}$ is self-adjoint and strictly positive, it has a well defined inverse. We may then take $G(\bar{f}, f') := \langle f, (\overline{K_R})^{-1} f'\rangle$, whenever this is a distribution. In an attempt to substantiate this procedure we will analyze the operator K_R in some more detail.

For a standard static space–time M we have $N^i \equiv 0 \equiv w$, so Eq. (4.4) simplifies to

$$N^{\frac{3}{2}} K N^{\frac{1}{2}} = \partial_0^2 + C_0 \,, \tag{6.2}$$

where C_0 is the partial differential operator

$$C_0 := -N^{\frac{1}{2}} \nabla_i^{(h)} N h^{ij} \nabla_j^{(h)} N^{\frac{1}{2}} + V N^2$$

acting on $C_0^\infty(\Sigma)$ in $L^2(\Sigma)$ (cf. Proposition 4.3). Recall from Subsec. 4.1 that the powers $\frac{3}{2}$ and $\frac{1}{2}$ of N to the left and right of K were chosen in such a way that C_0 is symmetric and at the same time the operator ∂_0^2 appears without any spatial dependence. In the case at hand that completely separates the Killing time dependence from the spatial dependence.

In a similar manner we may split off the imaginary Killing time dependence of K_R. For this we will view the circle $\mathbb{S}_R^1$ of radius R as a Riemannian manifold in the canonical metric $d\tau^2$. In analogy to the Lorentzian case (cf. Subsec. 4.1), there is a unitary isomorphism

$$U_R \colon L^2(M_R) \to L^2\big(\mathbb{S}_R^1\big) \otimes L^2(\Sigma) : f \mapsto \sqrt{N} f \,,$$

onto the Hilbert tensor product, because $d\,\mathrm{vol}_{g_R} = N d\tau\, d\,\mathrm{vol}_h$. Then, $N^{\frac{3}{2}} K_R N^{\frac{1}{2}} = -\partial_\tau^2 + C_0$, with the same operator C_0 on Σ as in the Lorentzian case. More precisely, we have

$$U_R N K_R N U_R^{-1} \supset B_R \otimes I + I \otimes C_0 \,, \tag{6.3}$$

where the operator $B_R := -\partial_\tau^2$ acts on the dense domain $C_0^\infty(\mathbb{S}_R^1)$ in $L^2(\mathbb{S}_R^1)$ and the operator on the right-hand side is defined on the algebraic tensor product of the domains of B_R and C_0.

The properties of the operator B_R are well known and we quote them without proof:

Proposition 6.1. *The operator $B_R := -\partial_\tau^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{S}_R^1)$ in $L^2(\mathbb{S}_R^1)$. If R is finite, there is a countable orthonormal basis of eigenvectors $\psi_n(\tau) := \frac{1}{\sqrt{2\pi R}} e^{in\tau/R}$, $n \in \mathbb{Z}$, with eigenvalues $\lambda_n := \frac{n^2}{R^2}$.*

This follows e.g. from Theorem II.9 in Ref. 21 by rescaling to $R = 1$. Note that for finite R the operator B_R is positive, but not strictly positive. From now on we will use B_R to denote the unique self-adjoint extension found in Proposition 6.1, to unburden our notation.

Together with the results for C (Proposition 4.3), Proposition 6.1 implies

Theorem 6.3. *For any $R > 0$ the operator NK_RN is essentially self-adjoint on $C_0^\infty(M_R)$ in $L^2(M_R)$, its closure is strictly positive with $NK_RN \geq VN^2$ and the domain of $(\overline{NK_RN})^{-\frac{1}{2}}$ contains $C_0^\infty(M_R)$.*

Proof. By Theorem VIII.33 in Ref. 21 the sum $B_R \otimes I + I \otimes C$ is essentially self-adjoint on the algebraic tensor product $\mathcal{D} := C_0^\infty(\mathbb{S}_R^1) \otimes C_0^\infty(\Sigma)$, because both B_R and C are essentially self-adjoint on the space of test-functions. By Eq. (6.3) the operator $U_RNK_RNU_R^{-1}$ extends $B_R \otimes I + I \otimes C$ and U_R is unitary, so NK_RN is already essentially self-adjoint on the smaller domain $U_R^{-1}\mathcal{D}$. In fact, because $\mathcal{D} \subset C_0^\infty(\mathbb{S}_R^1 \otimes \Sigma)$ in $L^2(\mathbb{S}_R^1 \otimes \Sigma, d\tau\, d\,\mathrm{vol}_h)$ we have $U_RNK_RNU_R^{-1} = B_R \otimes I + I \otimes C \geq I \otimes C \geq I \otimes VN^2$ on $\mathcal{D}$. It follows that $NK_RN \geq VN^2$ on $U_R^{-1}\mathcal{D}$ and hence on $C_0^\infty(M_R)$. The claim on the domain of $(\overline{NK_RN})^{-\frac{1}{2}}$ then follows from Lemma A.6 in the Appendix. □

In the ultra-static case, where N is constant, Theorem 6.3 (in combination with Theorem A.1) suffices to justify the procedure to define a Euclidean Green's function by $G_R(f, f') := \langle (\overline{K_R})^{-\frac{1}{2}} \bar{f}, (\overline{K_R})^{-\frac{1}{2}} f' \rangle$. In the general case, however, the study of the self-adjoint extensions of the operator K_R is more complicated.[n] Nevertheless, we can define a Euclidean Green's function by a slight modification of the common procedure as

$$G_R(f, f') := \left\langle (\overline{NK_RN})^{-\frac{1}{2}} N\bar{f}, (\overline{NK_RN})^{-\frac{1}{2}} Nf' \right\rangle, \tag{6.4}$$

[n]Some partial results are the following: (i) When $V = m^2 > 0$, K_R is essentially self-adjoint on $C_0^\infty(M_R)$ in $L^2(M_R)$ if and only if its range is dense, in which case its closure is strictly positive. For this to be the case it is sufficient that N^{-1} is bounded. (ii) If the Riemannian manifold (M_R, g_R) has a negligible boundary,[64] then K_R is essentially self-adjoint and its closure is strictly positive. Unfortunately, the boundedness of N^{-1} does not hold if the space–time is the exterior region of a black hole, while the condition in (ii) may only hold for very special choices of R.

using Theorem 6.3 and the fact that multiplication by N is a continuous linear map on $C_0^\infty(M)$. It is straightforward to verify that this satisfies all the requirements to be a Euclidean Green's function and we will see shortly that this choice of the Euclidean Green's function will indeed allow us to recover the KMS two-point distributions.

6.3.2. *Analytic continuation of the Euclidean Green's function*

We may now establish the explicit Killing time dependence of the Euclidean Green's function and its analytic continuation:

Theorem 6.4. *Consider a standard static globally hyperbolic space–time M. For each $R < \infty$ there is a unique continuous function $G_R^c(z,z')$ from $\mathcal{C}_R^{\times 2}$ into the distribution densities on $\Sigma^{\times 2}$, holomorphic on the set where $\mathrm{Im}(z-z') \neq 0$, such that for all χ, $\chi' \in C_0^\infty(\mathbb{S}_R^1)$ and f, $f' \in C_0^\infty(\Sigma)$ we have*

$$\langle U_R^{-1}(\chi \otimes f), G_R U_R^{-1}(\chi' \otimes f')\rangle = \int_{S_R^{\times 2}} d\tau\, d\tau'\, \bar{\chi}(\tau)\chi'(\tau')G_R^c(i\tau, i\tau'; \bar{f}, f')$$

with $z = t + i\tau$. When $\mathrm{Im}(z-z') \in [-2\pi R, 0]$ it is given by

$$G_R^c(z,z';\bar{f},f') := \left\langle C^{-\frac{1}{2}}Nf, \frac{\cos((z-z'+i\pi R)\sqrt{C})}{2\sinh(\pi R\sqrt{C})}Nf' \right\rangle.$$

Proof. It suffices to check that the given formula for G_R^c satisfies all the desired properties, but let us first sketch a more constructive argument to see where the formula comes from. When we try to extract the Killing time dependence of G_R, as defined in Eq. (6.4), we may make use of the fact that the inverse of the strictly positive operator $\overline{NK_RN}$ can be found as a strongly converging integral of the heat kernel,

$$\int_0^\infty d\alpha\, e^{-\alpha(\overline{NK_RN})}\psi = (\overline{NK_RN})^{-1}\psi\,, \tag{6.5}$$

for all $\psi \in D((\overline{NK_RN})^{-1})$. The importance of the heat kernel (i.e. the exponential function) is that it allows us to separate out the Killing time dependence. Indeed, for all $\alpha \geq 0$ there holds $e^{-\alpha(\overline{NK_RN})} = U_R^{-1}e^{-\alpha B_R} \otimes e^{-\alpha C}U_R$, because of Trotter's product formula (Ref. 21, Theorem VIII.31). Now let λ_n, $n \in \mathbb{Z}$, denote the eigenvalues of B_R and P_n the corresponding orthogonal projections. Then we may perform the integral over the heat kernel to find $U_R(\overline{NK_RN})^{-1}U_R^{-1}P_n = \overline{P_n \otimes (C+\lambda_n)^{-1}}$. Summing over n we then expect the formula

$$U_R(\overline{NK_RN})^{-1}U_R^{-1} = \sum_{n\in\mathbb{Z}} \frac{R}{2\pi} e^{i\frac{n}{R}(\tau-\tau')}(R^2C+n^2)^{-1}\,,$$

where we have written P_n as an integral kernel on $\left(\mathbb{S}^1_R\right)^{\times 2}$ and we substituted the values of λ_n. The sum over n can be performed (cf. Ref. 65, Formula 1.445:2) in the sense of the Spectral Calculus Theorem, leading to

$$U_R(\overline{NK_RN})^{-1}U_R^{-1} = \frac{\cosh((\tau-\tau'+\pi R)\sqrt{C})}{2\pi\sqrt{C}\sinh(\pi R\sqrt{C})}\,.$$

The analytic continuation is then obvious.

Let us now verify that the given formula for G^c_R has the desired properties. First note that for each z, z' with $\mathrm{Im}(z-z')\in[-2\pi R,0]$ it defines a distribution density on $\Sigma^{\times 2}$ by Theorem A.1, because multiplication by N is a continuous linear map from $C_0^\infty(\Sigma)$ to itself, $C_0^\infty(\Sigma)$ is in the domain of $C^{-\frac{1}{2}}$, by Proposition 4.3, and

$$\frac{\cos\big((\tau-\tau'+\pi R)\sqrt{C}\big)}{\sinh(\pi R\sqrt{C})} = \left(e^{(iz-iz'-2\pi R)\sqrt{C}} + e^{-i(z-z')\sqrt{C}}\right)\left(I-e^{-2\pi R\sqrt{C}}\right)^{-1},$$

by the Spectral Calculus Theorem. Moreover, both exponential terms in the first factor of the last expression are bounded operators that depend holomorphically on z, z' as long as $\mathrm{Im}(z-z')\in(-2\pi R,0)$. This proves the continuity and the holomorphicity claims. As the uniqueness of G^c_R is clear from the Edge of the Wedge Theorem,[23] it only remains to prove that it restricts to G_R.

For any f, $f'\in C_0^\infty(\Sigma)$ the function

$$G^c_R(i\tau,i\tau';\bar{f},f') = \tfrac{1}{2}\left\langle C^{-\frac{1}{2}}Nf, \left(e^{-(\tau-\tau'-2\pi R)\sqrt{C}} + e^{(\tau-\tau')\sqrt{C}}\right)\left(I-e^{-2\pi R\sqrt{C}}\right)^{-1}Nf'\right\rangle$$

is continuous for $\tau-\tau'\in[-2\pi R,0]$ and holomorphic in the interior. We may compute the derivatives in the distributional sense, which leads to

$$\begin{aligned}-\partial_\tau^2 G^c_R(i\tau,i\tau';\bar{f},f') &= -\partial_{\tau'}^2 G^c_R(i\tau,i\tau';\bar{f},f')\\ &= -G^c_R(i\tau,i\tau';N^{-1}CN\bar{f},f') + \delta(\tau-\tau')\langle Nf,Nf'\rangle\\ &= -G^c_R(i\tau,i\tau';\bar{f},N^{-1}CNf') + \delta(\tau-\tau')\langle Nf,Nf'\rangle\,.\end{aligned}$$

Letting $U_RK_RU_R^{-1} = N^{-1}(-\partial_\tau^2+C_0)N^{-1}$ act on $G^2_R(i\tau,i\tau';x,x')$ from the left and right we find

$$\begin{aligned}&-\partial_\tau^2 G^c_R(i\tau,i\tau';N^{-2}\bar{f},f') + G^c_R(i\tau,i\tau';N^{-1}CN^{-1}\bar{f},f')\\ &\quad= -\partial_{\tau'}^2 G^c_R(i\tau,i\tau';\bar{f},N^{-2}f') + G^c_R(i\tau,i\tau';\bar{f},N^{-1}CN^{-1}f') = \delta(\tau-\tau')\langle f,f'\rangle\,,\end{aligned}$$

which shows that the restriction of G^c_R to $\left(\mathbb{S}^1_R\right)^{\times 2}$ is indeed the Euclidean Green's function. □

The case $R=\infty$ can be treated using similar methods,[49] now using Ref. 65, Formula 3.472:5. The result is the distribution density-valued function

$$G^c_\infty(z,z';\bar{f},f') := \frac{1}{2}\left\langle C^{-\frac{1}{2}}Nf, e^{-i(z-z')\sqrt{C}}Nf'\right\rangle.$$

Alternatively, this expression can be obtained as the limit

$$G^c_\infty(z,z';\bar{f},f') = \lim_{R\to\infty} G^c_R(z,z';\bar{f},f')\,,$$

for fixed f, $f' \in C_0^\infty(\Sigma)$, using Lemma A.8.

6.3.3. *Wick rotation to fundamental solutions and thermal states*

Using the analytic continuation G^c_R we now want to complete the Wick rotation by considering the restriction to real values $z = t$ and $z' = t'$. Following Ref. 5 we show how the thermal two-point distribution and the advanced, retarded and Feynman fundamental solutions are obtained.

Both for $t > t'$ and $t < t'$ we can approach the real axis from above, $\mathrm{Im}(z-z') > -2\pi R$, and from below, $\mathrm{Im}(z-z') < 0$. This prompts us to define the following functions on $\mathbb{R}^{\times 2}$ with values in the distribution densities on $\Sigma^{\times 2}$:

$$\begin{aligned}
\mathscr{E}^+(t,t';f,f') &:= i\theta(t-t')\big(G^c_R(t,t';f,f') - G^c_R(t-2\pi iR,t';f,f')\big)\\
\mathscr{E}^-(t,t';f,f') &:= -i\theta(t'-t)\big(G^c_R(t,t';f,f') - G^c_R(t-2\pi iR,t';f,f')\big)\\
\mathscr{E}^F_R(t,t';f,f') &:= i\theta(t-t')G^c_R(t,t';f,f') + i\theta(t'-t)G^c_R(t-2\pi iR,t';f,f')\,.
\end{aligned}$$

Note that the $\mathscr{E}^\pm$ and $\mathscr{E}^F_R$ are given by

$$\begin{aligned}
\mathscr{E}^\pm(t,t';\bar{f},f') &= \pm\theta(\pm(t-t'))\Big\langle C^{-\frac{1}{2}}Nf, \sin\big((t-t')\sqrt{C}\big)Nf'\Big\rangle\,,\\
\mathscr{E}^F_R(t,t';\bar{f},f') &= i\Big\langle C^{-\frac{1}{2}}Nf, \frac{\cos((|t-t'|+i\pi R)\sqrt{C})}{2\sin(\pi R\sqrt{C})}Nf'\Big\rangle\,.
\end{aligned} \tag{6.6}$$

They give rise to distribution densities on $M^{\times 2}$ defined by

$$\begin{aligned}
E^\pm(\chi\otimes f,\chi'\otimes f') &:= \int dt\,dt'\,\chi(t)\chi'(t')\mathscr{E}^\pm\big(t,t';\sqrt{N}f,\sqrt{N}f'\big)\,,\\
E^F_R(\chi\otimes f,\chi'\otimes f') &:= \int dt\,dt'\,\chi(t)\chi'(t')\mathscr{E}^F_R\big(t,t';\sqrt{N}f,\sqrt{N}f'\big)
\end{aligned} \tag{6.7}$$

and using Schwartz Kernels Theorem to extend the distribution to all test-functions in $C_0^\infty(M)$. (Note that the factors $\sqrt{N}$ are required to account for the change in integration measure and they can equivalently be written in terms of the unitary isomorphism U.)

Proposition 6.2. *$E^\pm$ and E^F_R are left and right fundamental solutions for the Klein–Gordon operator $K = -\Box + V$ and we have $\mathscr{E}^\pm(t,t';f,f') = \mathscr{E}^\mp(t',t;f,f') = \overline{\mathscr{E}^\pm(t,t';\bar{f},\overline{f'})} = \mathscr{E}^\pm(t,t';f',f)$.*

Proof. The first sequence of equalities follows directly from Eq. (6.6) and the fact that $L^2(\Sigma)$ carries a natural complex conjugation which commutes with the operator C and any real-valued function of C. To see that the distribution densities are fundamental solutions we use Eq. (6.2) to find

$$UKU^{-1}(\chi \otimes f) = \chi \otimes N^{-1}CN^{-1}f + \partial_t^2\chi \otimes N^{-2}f$$

and we use the fact that

$$\partial_t^2 G_R^c(t,t';N^{-2}f,f') + G_R^c(t,t';N^{-1}CN^{-1}f,f') = 0\,.$$

(The differentiations can be carried out by going into the complex manifold M^c, where G_R^c is holomorphic, and then extending by continuity to the boundary.) For the case of $E^{\pm}(t,t')$ we then have, by Eq. (6.6):

$$\begin{aligned}
&((K\otimes I)E^{\pm})(U^{-1}(\chi\otimes f), U^{-1}(\chi'\otimes f'))\\
&\quad = E^{\pm}(U^{-1}(\chi\otimes N^{-1}CN^{-1}f), U^{-1}(\chi'\otimes f'))\\
&\qquad + E^{\pm}(U^{-1}(\partial_t^2\chi\otimes N^{-2}f), U^{-1}(\chi'\otimes f'))\\
&\quad = \pm\int dt\,dt'\,\chi(t)\chi'(t')\theta(\pm(t-t'))\left\langle\sqrt{C}N^{-1}\bar{f}, \sin((t-t')\sqrt{C})Nf'\right\rangle\\
&\qquad + \partial_t^2\chi(t)\chi'(t')\theta(\pm(t-t'))\left\langle C^{-\frac{1}{2}}N^{-1}\bar{f}, \sin((t-t')\sqrt{C})Nf'\right\rangle.
\end{aligned}$$

We account for the factors θ by restricting the domain of integration and then perform partial integrations, after which we are only left with the boundary terms, which immediately yield the result. By the symmetry properties of $\mathscr{E}^{\pm}$, $E^{\pm}$ is also a right-fundamental solution. The proof for E_R^F uses a similar computation. $\square$

It follows from the support properties of the distribution densities $E^{\pm}$ that they are the advanced $(-)$ and retarded $(+)$ fundamental solutions, so our notation is consistent. As Eq. (6.6) shows, they are independent of R, in line with the uniqueness of these fundamental solutions. E_R^F is the Feynman fundamental solution, as can be inferred from the fact that the real axis of $t-t'$ is approached by a rigid rotation from the imaginary time axis in counterclockwise direction. It does depend on the choice of R and it defines a choice of two-point distribution as follows:

Proposition 6.3. *For $0 < R < \infty$ the function $G_R^c(t,t') = -i(\mathscr{E}_R^F - \mathscr{E}^-)(t,t')$ on $\mathbb{R}^{\times 2}$ has a corresponding distribution density $\omega_2^{(\beta)} := -i(E_R^F - E^-)$ where we set $\beta := 2\pi R$. $\omega_2^{(\beta)}$ is the two-point distribution density of $\omega^{(\beta)}$ (as defined in Theorem* 6.2) *and*

$$\begin{aligned}
&\omega_2^{(\beta)}(U^{-1}(\chi\otimes f), U^{-1}(\chi'\otimes f'))\\
&\quad = \int dt\,dt'\,\chi(t)\chi'(t')G_R^c(t,t';f,f')\\
&\quad = \int dt\,dt'\,\chi(t)\chi'(t')\left\langle C^{-\frac{1}{2}}v\bar{f}, \frac{\cos((t-t'+i\pi R)\sqrt{C})}{2\sinh(\pi R\sqrt{C})}vf'\right\rangle.
\end{aligned}$$

Proof. The equality $G^c_R(t,t') = -i(\mathscr{E}^F_R - \mathscr{E}^-)(t,t')$ follows directly from the definitions of G^c_R, $\mathscr{E}^F_R$ and $\mathscr{E}^-$, so it remains to check the properties of $\omega_2^{(\beta)}$. $\omega_2^{(\beta)}$ is a bisolution to the Klein–Gordon equation because it is $-i$ times a difference of two fundamental solutions (Proposition 6.2). Furthermore, comparison with Eqs. (6.6) and (6.7) shows that the antisymmetric part of $\omega_2^{(\beta)}$ is given by $\frac{i}{2}(E^- - E^+)$. Remembering that $\partial_t = Nn^a\nabla_a$ and that the restriction of a distribution density from M to Σ incurs a factor N^{-1} we find that the initial data of $\omega_2^{(\beta)}$ are given by

$$\begin{aligned} \omega^{(\beta)}_{2,00}(\bar{f}_1, f'_1) &= \frac{1}{2}\left\langle C^{-\frac{1}{2}}N^{\frac{1}{2}}f_1, \coth\left(\frac{\beta}{2}C^{\frac{1}{2}}\right)N^{\frac{1}{2}}f'_1\right\rangle, \\ \omega^{(\beta)}_{2,10}(\bar{f}, f') &= \frac{-i}{2}\langle f, f'\rangle = -\omega^{(\beta)}_{2,01}(\bar{f}, f'), \\ \omega^{(\beta)}_{2,11}(\bar{f}_0, f'_0) &= \frac{1}{2}\left\langle C^{\frac{1}{2}}N^{-\frac{1}{2}}f_0, \coth\left(\frac{\beta}{2}C^{\frac{1}{2}}\right)N^{-\frac{1}{2}}f'_0\right\rangle. \end{aligned} \tag{6.8}$$

On the other hand, the nondegenerate β-KMS one-particle structure, which is described in Proposition 4.3 for the standard static case, defines a two-point distribution whose initial data coincide with those in Eq. (6.8), as one may verify by a short computation. This proves that $\omega_2^{(\beta)}$, as defined above, is indeed the two-point distribution of $\omega^{(\beta)}$. □

Using similar techniques one may treat the case $R = \infty$, which leads to the two-point distribution ω^0_2 of the ground state ω^0 of Theorem 5.1.[49]

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Appendix. Some Useful Results from Functional Analysis

In this appendix we collect some results from functional analysis, to make our review self-contained. Most of the proofs are omitted, because they are elementary or make use of standard methods. For more information we refer the reader to Refs. 15, 21 and 38 for strictly positive operators. In particular these references contain a detailed formulation of the Spectral Calculus Theorem (Ref. 15, Sec. 5.6 or Ref. 21, Theorem VIII.6).

If $X : \mathcal{H}_1 \to \mathcal{H}_2$ is a linear operator between two Hilbert spaces $\mathcal{H}_i$, we denote the domain of X by $D(X)$. We wish to record the following useful relation between operators on a Hilbert space and distributions.

Theorem A.1. *Let $X : \mathcal{H}_1 \to \mathcal{H}_2$ be a closed, densely defined linear operator between two Hilbert spaces $\mathcal{H}_i$ and let $L : C^\infty_0(M) \to \mathcal{H}_1$ be an $\mathcal{H}_1$-valued distribution* *density. If the range of L is contained in $D(X)$, then $f \mapsto XL(f)$ is an $\mathcal{H}_2$-valued distribution density.*

Proof. If X is a bounded operator this is immediately clear from $\|XL(f)\| \leq \|X\| \cdot \|L(f)\|$. If X is a self-adjoint operator on $\mathcal{H}_1 = \mathcal{H}_2$ we may use its spectral projections $P_{(-n,n)}$ onto the intervals $(-n, n)$ to define bounded operators $X_n := P_{(-n,n)}X$ for $n \in \mathcal{N}$. Each X_nL defines a distribution density and $\lim_{n\to\infty} X_nL(f) = XL(f)$ for all $f \in C_0^\infty(M)$, because $L(f) \in D(X)$. From the Uniform Bounded Principle (Ref. 21, Theorem III.9) we see that XL also defines an $\mathcal{H}_2$-valued distribution density. The general case now follows from the polar decomposition, Theorem 6.1.11 of Ref. 15, which allows us to write $T = V(T^*T)^{\frac{1}{2}}$, where V is bounded and $(T^*T)^{\frac{1}{2}}$ is a self-adjoint operator on $\mathcal{H}_1$ with the same domain as T. □

We now turn to injective (and therefore invertible) operators on a Hilbert space, starting with the following four general Lemmas:

Lemma A.1. *A densely defined, closable and injective operator X in a Hilbert space $\mathcal{H}$ has an injective closure $\bar{X}$ if and only if X^{-1} is closable.*

Lemma A.2. *If X is a densely defined, injective operator with dense range, then X^* and $(X^{-1})^*$ are injective and $(X^*)^{-1} = (X^{-1})^*$.*

Lemma A.3. *A self-adjoint operator X is invertible if and only if it has a dense range on any core.*

Lemma A.4. *If X is self-adjoint and invertible, then X^{-1} is self-adjoint and invertible, where the domain of X^{-1} is the range of X. If $\mathcal{D}$ is a core for X, then $X\mathcal{D}$ is a core for X^{-1}.*

These Lemmas can be proved using entirely elementary methods.

As positive invertible operators are particularly useful we make the following definition.

Definition A.1. A densely defined operator X in a Hilbert space $\mathcal{H}$ is called *strictly positive* if and only if X is self-adjoint and for any $0 \neq \phi \in D(X)$: $\langle \phi, X\phi \rangle > 0$.

Several equivalent characterizations can be given as follows:

Lemma A.5. *For a positive, self-adjoint operator X the following are equivalent:*

(i) *X is strictly positive.*
(ii) *X is injective.*
(iii) *X has a dense range on any core.*
(iv) *X^{-1} is strictly positive.*

Proof. (i) is equivalent to (iv) by Lemma A.4, because $\langle\phi, X^{-1}\phi\rangle = \langle X\psi, \psi\rangle$ when $\phi := X\psi$. The implication (i) $\Rightarrow$ (ii) is immediate and (ii) is equivalent to (iii) by Lemma A.3. To see that (ii) implies (i) one uses the Spectral Calculus Theorem and the fact that $\langle\phi, X\phi\rangle = 0$ implies $X^{\frac{1}{2}}\phi = 0$ and $X\phi = 0$. If X is injective, this means that $\phi = 0$. □

The following estimate is often useful to find strictly positive operators, in particular in combination with Lemma A.7 below.

Lemma A.6. *Let X and Y be positive self-adjoint operators with X strictly positive and assume that $Y \geq X$ on a core for $Y^{\frac{1}{2}}$. Then Y is strictly positive, $D\big(Y^{-\frac{1}{2}}\big) \supset D\big(X^{-\frac{1}{2}}\big)$ and $Y^{-1} \leq X^{-1}$ on $D\big(X^{-\frac{1}{2}}\big)$.*

Proof. Let $\mathcal{D}$ denote the core for $Y^{\frac{1}{2}}$ on which the estimate holds. The estimate $\big\|X^{\frac{1}{2}}\psi\big\| \leq \big\|Y^{\frac{1}{2}}\psi\big\|$ for $\psi \in \mathcal{D}$ can be extended to the entire domain $D\big(Y^{\frac{1}{2}}\big)$. Because X is strictly positive the same must be true for Y by Lemma A.5. By Lemma A.4, $\big\|X^{\frac{1}{2}}Y^{-\frac{1}{2}}\psi\big\| \leq \|\psi\|$ on $D\big(Y^{-\frac{1}{2}}\big)$. Note in particular that the range of $Y^{-\frac{1}{2}}$ is contained in $D\big(X^{\frac{1}{2}}\big)$. As $X^{\frac{1}{2}}Y^{-\frac{1}{2}}$ is bounded on $D\big(Y^{-\frac{1}{2}}\big)$ we also find that the range of $X^{\frac{1}{2}}$, which is $D\big(X^{-\frac{1}{2}}\big)$, is contained in the domain of $\big(Y^{-\frac{1}{2}}\big)^* = Y^{-\frac{1}{2}}$. It now follows that $\big(X^{\frac{1}{2}}Y^{-\frac{1}{2}}\big)^* = Y^{-\frac{1}{2}}X^{\frac{1}{2}}$ on $D\big(X^{\frac{1}{2}}\big)$. As $\big\|X^{\frac{1}{2}}Y^{-\frac{1}{2}}\big\| \leq 1$ we must also have $\big\|Y^{-\frac{1}{2}}X^{\frac{1}{2}}\big\| \leq 1$, which implies that $\big\|Y^{-\frac{1}{2}}\psi\big\| \leq \big\|X^{-\frac{1}{2}}\psi\big\|$ on $D\big(X^{-\frac{1}{2}}\big)$ and the conclusion follows. □

Lemma A.7. *Let $X \geq 0$ be a densely defined, positive operator. Then the Friedrichs extension $\hat{X}$ is positive and $D(X)$ is a core for $\hat{X}^{\frac{1}{2}}$.*

The following lemma concerns the heat kernel:

Lemma A.8. *Let X be a positive self-adjoint operator on $\mathcal{H}$ and let $\mathbb{C}_+ := \{z \in \mathbb{C} \,|\, \mathrm{Re}(z) > 0\}$ be the right half space. Then the function $z \mapsto e^{-zX}$ is holomorphic on $\mathbb{C}_+$ with values in the bounded operators on $\mathcal{H}$ and for each $\psi \in \mathcal{H}$ the function $e^{-zX}\psi$ is continuous on $\overline{\mathbb{C}_+}$.*

To close this appendix we provide some facts concerning multiplication operators on the L^2 space of a semi-Riemannian manifold:

Proposition A.1. *Let (M, g) be an orientable semi-Riemannian manifold, let $w \in C^\infty(M)$ and let W be the corresponding multiplication operator in $L^2(M, d\,\mathrm{vol}_g)$, defined on $C_0^\infty(M)$ by $(Wf)(x) = w(x)f(x)$. If $|w|$ is bounded, then W is bounded. If w is real-valued, then W is essentially self-adjoint. $\bar{W}$ is (strictly) positive if and only if w is (strictly) positive (almost everywhere).*

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