Microlocal Analysis of Quantum Fields on Curved Spacetimes

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CHAPTER 1

Introduction

1.1. Introduction

Quantum Field Theory arose from the need to unify Quantum Mechanics with special relativity. It is usually formulated on the flat Minkowski spacetime, on which classical field equations, such as the Klein-Gordon, Dirac or Maxwell equations are easily defined. Their quantization rests on the so-called *Minkowski vacuum*, which describes a state of the quantum field containing no particles. The Minkowski vacuum is also fundamental for the perturbative or non-perturbative construction of interacting theories, corresponding to the quantization of non-linear classical field equations.

Quantum Field Theory on Minkowski spacetime relies heavily on its symmetry under the Poincaré group. This is apparent in the ubiquitous role of plane waves in the analysis of classical field equations, but more importantly in the characterization of the Minkowski vacuum as the unique state which is invariant under the Poincaré group and has some *energy positivity* property.

Quantum Field Theory on *curved spacetimes* describes quantum fields in an external gravitational field, represented by the Lorentzian metric of the ambient spacetime. It is used in situations when both the quantum nature of the fields and the effect of gravitation are important, but the quantum nature of gravity can be neglected in a first approximation. Its non-relativistic analog would be for example ordinary Quantum Mechanics, i.e. the Schrödinger equation, in a classical exterior electromagnetic field.

Its most important areas of application are the study of phenomena occurring in the early universe and in the vicinity of black holes, and its most celebrated result is the discovery by Hawking that quantum particles are created near the horizon of a black hole.

The symmetries of the Minkowski spacetime, which play such a fundamental role, are absent in curved spacetimes, except in some simple situations, like *stationary* or *static* spacetimes. Therefore, the traditional approach to quantum field theory has to be modified: one has first to perform an *algebraic quantization*, which for free theories amounts to introducing an appropriate *phase space*, which is either a *symplectic* or an *Euclidean* space, in the *bosonic* or *fermionic* case. From such a phase space one can construct CCR or CAR $*$-*algebras*, and actually *nets* of $*$-algebras, each associated to a region of spacetime.

The second step consists in singling out, among the many states on these $*$-algebras, the physically meaningful ones, which should resemble the Minkowski vacuum, at least in the vicinity of any point of the spacetime. This leads to the notion of *Hadamard states*, which were originally defined by requiring that their two-point functions have a specific asymptotic expansion near the diagonal, called the *Hadamard expansion*.

A very important progress was made by Radzikowski, [**R1, R2**], who introduced the characterization of Hadamard states by the *wavefront set* of their two-point functions. The wavefront set of a distribution is the natural way to describe

its singularities in the cotangent space, and lies at the basis of *microlocal analysis*, a fundamental tool in the analysis of linear and non-linear partial differential equations. Among its avatars in the physics literature are, for example, the geometrical optics in wave propagation and the semi-classical limit in Quantum Mechanics.

The introduction of microlocal analysis in quantum field theory on curved spacetimes started a period of rapid progress, non only for free (i.e. linear) quantum fields, but also for the perturbative construction of interacting fields by Brunetti and Fredenhagen [**BF**]. For free fields it allowed to use several fundamental results of microlocal analysis, like Hörmander's propagation of singularities theorem and the classification of parametrices for Klein-Gordon operators by Duistermaat and Hörmander.

1.2. Content

The goal of these lecture notes is to give an exposition of microlocal analysis methods in the study of Quantum Field Theory on curved spacetimes. We will focus on *free fields* and the corresponding *quasi-free states* and more precisely on *Klein-Gordon fields*, obtained by quantization of linear Klein-Gordon equations on Lorentzian manifolds, although the case of *Dirac fields* will be described in Chapter 17.

There exist already several good textbooks or lecture notes on quantum field theory in curved spacetimes. Among them let us mention the book by Bär, Ginoux and Pfaeffle [**BGP**], the lecture notes [**BFr**] and [**BDFY**], the more recent book by Rejzner [**Re**], and the survey by Benini, Dappiagi and Hack [**BDH**]. There exist also more physics oriented books, like the books by Wald [**W2**], Fulling [**F**] and Birrell and Davies [**BD**]. Several of these texts contain important developments which are not described here, like the perturbative approach to interacting theories, or the use of category theory.

In this lecture notes we focus on advanced methods from microlocal analysis, like for example *pseudodifferential calculus*, which turn out to be very useful in the study and construction of Hadamard states.

Pure mathematicians working in partial differential equations are often deterred by the traditional formalism of quantum field theory found in physics textbooks, and by the fact that the construction of interacting theories is, at least for the time being, restricted to perturbative methods.

We hope that these lecture notes will convince them that quantum field theory on curved spacetimes is full of interesting and physically important problems, with a nice interplay between algebraic methods, Lorentzian geometry and microlocal methods in partial differential equations. On the other hand, mathematical physicists with a traditional education, which may lack familiarity with more advanced tools of microlocal analysis, can use this text as an introduction and motivation to the use of these methods.

Let us now give a more detailed description of these lecture notes. The reader may also consult the introduction of each chapter for more information.

For pedagogical reasons, we have chosen to devote Chapters 2 and 3 to a brief outline of the traditional approach to quantization of Klein-Gordon fields on Minkowski spacetime, but the impatient reader can skip them without trouble.

Chapter 4 deals with CCR $*$-algebras and quasi-free states. A reader with a PDE background may find the reading of this chapter a bit tedious. Nevertheless, we think it is worth the effort to get familiar with the notions introduced there.

In Chapter 5 we describe well-known concepts and results concerning Lorentzian manifolds and Klein-Gordon equations on them. The most important are the notion

of *global hyperbolicity*, a property of a Lorentzian manifold implying global solvability of the Cauchy problem, and the *causal propagator* and the various symplectic spaces associated to it.

In Chapter 6 we discuss quasi-free states for Klein-Gordon fields on curved spacetimes, which is a concrete application of the abstract formalism in Chapter 4. Of interest are the two possible descriptions of a quasi-free state, either by it spacetime covariances, or by its Cauchy surface covariances, which are both important in practice. Another useful point is the discussion of conformal transformations.

Chapter 7 is devoted to the microlocal analysis of Klein-Gordon equations. We collect here various well-known results about wavefront sets, Hörmander's propagation of singularities theorem and its related study with Duistermaat of *distinguished parametrices* for Klein-Gordon operators, which play a fundamental role in quantized Klein-Gordon fields.

In Chapter 8 we introduce the modern definition of Hadamard states due to Radzikowski and discuss some of its consequences. We explain the equivalence with the older definition based on Hadamard expansions and the well-known existence result by Fulling, Narcowich and Wald.

In Chapter 9 we discuss ground states and thermal states, first in an abstract setting, then for Klein-Gordon operators on stationary spacetimes. Ground states share the symmetries of the background stationary spacetime and are the natural analogs of the Minkowski vacuum. In particular, they are the simplest examples of Hadamard states.

Chapter 10 is devoted to an exposition of a global pseudodifferential calculus on non compact manifolds, the *Shubin calculus*. This calculus is based on the notion of manifolds of bounded geometry and is a natural generalization of the standard uniform calculus on $\mathbb{R}^n$. Its most important properties are the Seeley and Egorov theorems.

In Chapter 11 we explain the construction of Hadamard states using the pseudodifferential calculus in Chapter 10. The construction is done, after choosing a Cauchy surface, by a microlocal splitting of the space of Cauchy data obtained from a global construction of parametrices for the Cauchy problem. It can be applied to many spacetimes of physical interest, like the Kerr-Kruskal and Kerr-de Sitter spacetimes.

In Chapter 12 we construct *analytic* Hadamard states by *Wick rotation*, a well-known procedure in Minkowski spacetime. Analytic Hadamard states are defined on analytic spacetimes, by replacing the usual C^∞ wavefront set by the *analytic wavefront set*, which describes the analytic singularities of distributions. Like the Minkowski vacuum, they have the important *Reeh-Schlieder* property. After Wick rotation, the hyperbolic Klein-Gordon operator becomes an elliptic Laplace operator, and analytic Hadamard states are constructed using a well-known tool from elliptic boundary value problems, namely the *Calderón projector*.

In Chapter 13 we describe the construction of Hadamard states by the *characteristic Cauchy problem*. This amounts to replacing the space-like Cauchy surface in Chapter 11 by a past or future *lightcone*, choosing its interior as the ambient spacetime. From the trace of solutions on this cone one can introduce a *boundary symplectic space*, and it turns out that it is quite easy to characterize states on this symplectic space which generate a Hadamard state in the interior. Its main application is the *conformal wave equation* on spacetimes which are asymptotically flat at past or future *null infinity*. We also describe in this chapter the BMS *group* of asymptotic symmetries of these spacetimes, and its relationship with Hadamard states.

In Chapter 14 we discuss Klein-Gordon fields on spacetimes with Killing horizons. Our aim is to explain a phenomenon loosely related with the *Hawking radiation*, namely the existence of the *Hartle-Hawking-Israel* vacuum, on spacetimes having a stationary Killing horizon. The construction and properties of this state follow from the Wick rotation method already used in Chapter 12, the Calderón projectors playing also an important role.

Chapter 15 is devoted to the construction of Hadamard states by scattering theory methods. We consider spacetimes which are asymptotically static at past or future time infinity. In this case one can define the *in* and *out vacuum states*, which are states asymptotic to the vacuum state at past or future time infinity. Using the tools from Chapters 10, 11 we prove that these states are Hadamard states.

In Chapter 16 we discuss the notion of *Feynman inverses*. It is known that a Klein-Gordon operator on a globally hyperbolic spacetime admits *Feynman parametrices*, which are unique modulo smoothing operators and characterized by the wavefront set of its distributional kernels. One can ask if one can also define a unique, canonical true inverse, having the correct wavefront set. We give a positive answer to this question on spacetimes which are *asymptotically Minkowski*.

Chapter 17 is devoted to the quantization of the *Dirac equation* and to the definition of Hadamard states for Dirac quantum fields. The Dirac equation on a curved spacetime describes an electron-positron field which is a *fermionic* field, and the CCR $*$-algebra for the Klein-Gordon field has to be replaced by a CAR $*$-algebra. Apart from this difference, the theory for fermionic fields is quite parallel to the bosonic case. We also describe the quantization of the *Weyl equation*, which originally was thought to describe massless neutrinos.

1.2.1. Acknowledgments. The results described in Chapters 11, 12, 15, and part of those in Chapters 10 and 13, originate from common work with Michal Wrochna, over a period of several years.

I learned a lot of what I know about quantum field theory from my long collaboration with Jan Derezinski, and several parts of these lecture notes, like Chapters 4 and 5 borrow a lot from our common book [**DG**]. I take the occasion here to express my gratitude to him.

Finally, I also greatly profited from discussions with members of the AQFT community. Among them I would like to especially thank Claudio Dappiagi, Valter Moretti, Nicola Pinamonti, Igor Khavkine, Klaus Fredenhagen, Detlev Bucholz, Wojciech Dybalski, Kasia Rejzner, Dorothea Bahns, Rainer Verch, Stefan Hollands and Ko Sanders.

1.3. Notation

We now collect some notation that we will use.

We set $\langle\lambda\rangle = (1+\lambda^2)^{\frac{1}{2}}$ for $\lambda \in \mathbb{R}$.

We write $A \Subset B$ if A is relatively compact in B.

If X, Y are sets and $f : X \to Y$ we write $f : X \xrightarrow{\sim} Y$ if f is bijective. If X, Y are equipped with topologies, we write $f : X \to Y$ if the map is continuous, and $f : X \xrightarrow{\sim} Y$ if it is a homeomorphism.

1.3.1. Scale of abstract Sobolev spaces. Let $\mathcal{H}$ a real or complex Hilbert space and A a selfadjoint operator on $\mathcal{H}$. We write $A > 0$ if $A \geq 0$ and $\operatorname{Ker} A = \{0\}$.

If $A > 0$ and $s \in \mathbb{R}$, we equip $\operatorname{Dom} A^{-s}$ with the scalar product $(u|v)_{-s} = (A^{-s}u|A^{-s}v)$ and the norm $\|A^{-s}u\|$. We denote by $A^s\mathcal{H}$ the completion of $\operatorname{Dom} A^{-s}$ for this norm, which is a (real or complex) Hilbert space.

CHAPTER 2

Free Klein-Gordon fields on Minkowski spacetime

Almost all textbooks on quantum field theory start with the quantization of the free (i.e. linear) Klein-Gordon and Dirac equations on Minkowski spacetime. The traditional exposition rests on the so-called *frequency splitting*, which amounts to splitting the space of solutions of, say, the Klein-Gordon equation into two subspaces, corresponding to solutions having positive/negative energy, or equivalently whose Fourier transforms are supported in the upper/lower mass hyperboloid.

One then proceeds with the introduction of *Fock spaces* and the definition of quantized Klein-Gordon or Dirac fields using *creation/annihilation operators*.

Since it relies on the use of the Fourier transformation, this method does not carry over to Klein-Gordon fields on curved spacetimes. More fundamentally, it has the drawback of mixing two different steps in the quantization of the Klein-Gordon equation.

The first, purely algebraic step consists in using the symplectic nature of the Klein-Gordon equation to introduce an appropriate CCR $*$-*algebra*. The second step consists in choosing a *state* on this algebra, which on the Minkowski spacetime is the *vacuum state*.

Nevertheless it is useful to keep in mind the Minkowski spacetime as an important example. This chapter is devoted to the classical theory of the Klein-Gordon equation on Minkowski spacetime, i.e. to its symplectic structure. Its Fock quantization will be described in Chapter 3.

2.1. Minkowski spacetime

In the sequel we will use notation introduced later in Section 4.1.

The elements of $\mathbb{R}^n = \mathbb{R}_t \times \mathbb{R}^d_{\mathrm{x}}$ will be denoted by $x = (t, \mathrm{x})$, those of the dual $(\mathbb{R}^n)'$ by $\xi = (\tau, \mathrm{k})$.

2.1.1. The Minkowski spacetime.

Definition 2.1.1. *The* Minkowski spacetime $\mathbb{R}^{1,d}$ *is* $\mathbb{R}^{1+d}$ *equipped with the bilinear form* $\eta \in L_{\mathrm{s}}(\mathbb{R}^{1+d}, (\mathbb{R}^{1+d})')$ *given by*

$$x \cdot \eta x = -t^2 + \mathrm{x}^2. \tag{2.1}$$

Definition 2.1.2. (1) *A vector* $x \in \mathbb{R}^{1,d}$ *is* time-like *if* $x \cdot \eta x < 0$, null *if* $x \cdot \eta x = 0$, causal *if* $x \cdot \eta x \leq 0$, *and* space-like *if* $x \cdot \eta x > 0$.

(2) $C_\pm := \{x \in \mathbb{R}^{1,d} : \ x \cdot \eta x < 0, \ \pm t > 0\}$, *resp.* $\overline{C}_\pm := \{x \in \mathbb{R}^{1,d} : \ x \cdot \eta x \leq 0, \ \pm t \geq 0\}$ *are called the* open, *resp.* closed future/past (solid) lightcones.

(3) $N := \{x \in \mathbb{R}^{1,d} : x \cdot \eta x = 0\}$, *resp.* $N_\pm = N \cap \{\pm t \geq 0\}$ *are called the* null cone *resp.* future/past null cones.

There is a similar classification of vector subspaces of $\mathbb{R}^{1,d}$.

Definition 2.1.3. *A linear subspace* V *of* $\mathbb{R}^{1,d}$ *is* time-like *if it contains both space-like and time-like vectors,* null *if it is tangent to the null cone* N *and* space-like *if it contains only space-like vectors.*

DEFINITION 2.1.4. (1) *If* $K \subset \mathbb{R}^{1,d}$, $I_\pm(K) := K + C_\pm$, *resp.* $J_\pm(K) := K + \overline{C}_\pm$, *is called the* time-like, *resp.* causal future/past *of* K, *and* $J(K) := J_+(K) \cup J_-(K)$ *the* causal shadow *of* K.

(2) *Two sets* K_1, K_2 *are called* causally disjoint *if* $K_1 \cap J(K_2) = \emptyset$ *or, equivalently, if* $J(K_1) \cap K_2 = \emptyset$.

(3) *A function* f *on* $\mathbb{R}^n$ *is called* space-compact, *resp.* future/past space-compact, *if* $\operatorname{supp} f \subset J(K)$, *resp.* $\operatorname{supp} f \subset J_\pm(K)$ *for some compact set* $K \Subset \mathbb{R}^n$. *The spaces of smooth such functions will be denoted by* $C^\infty_{\mathrm{sc}}(\mathbb{R}^n)$, *resp.* $C^\infty_{\mathrm{sc},\pm}(\mathbb{R}^n)$.

2.1.2. The Lorentz and Poincaré groups.

DEFINITION 2.1.5. (1) *The pseudo-Euclidean group* $O(\mathbb{R}^{1+d}, \eta)$ *is denoted by* $O(1,d)$ *and is called the* Lorentz group.

(2) $SO(1,d)$ *is the subgroup of* $L \in O(1,d)$ *with* $\det L = 1$.

(3) *If* $L \in O(1,d)$ *one has* $L(J_+) = J_+$ *or* $L(J_+) = J_-$. *In the first case* L *is called* orthochronous *and in the second* anti-orthochronous.

(4) *The subgroup of orthochronous elements of* $SO(1,d)$ *is denoted by* $SO^\uparrow(1,d)$ *and called the* restricted Lorentz group.

DEFINITION 2.1.6. *The* (*restricted*) Poincaré group *is the set* $P(1,d) := \mathbb{R}^n \times SO^\uparrow(1,d)$ *equipped with the product*

$$(a_2, L_2) \times (a_1, L_1) = (a_2 + L_2 a_1, L_2 L_1).$$

The Poincaré group acts on $\mathbb{R}^n$ *by* $\Lambda x := Lx + a$ *for* $\Lambda = (a, L) \in P(1,d)$.

2.2. The Klein-Gordon equation

We recall that the differential operator

$$P = -\Box + m^2 := \partial_t^2 - \sum_{i=1}^d \partial_{x^i}^2 + m^2,$$

for $m \geq 0$ is called the *Klein-Gordon operator*.

We set $\epsilon(\mathrm{k}) = (k^2 + m^2)^{\frac{1}{2}}$ and denote by $\epsilon = \epsilon(D_{\mathrm{x}})$ the Fourier multiplier defined by $\mathcal{F}(\epsilon u)(\mathrm{k}) = \epsilon(\mathrm{k}) u(\mathrm{k})$, where $\mathcal{F}u(\mathrm{k}) = (2\pi)^{-d/2} \int \mathrm{e}^{-\mathrm{ik}\cdot\mathrm{x}} u(\mathrm{x}) d\mathrm{x}$ is the (unitary) Fourier transform. Note that $-\Box + m^2 = \partial_t^2 + \epsilon^2$.

The *Klein-Gordon equation*

$$-\Box\phi + m^2\phi = 0 \tag{2.2}$$

is the simplest relativistic field equation. Its quantization describes a *scalar bosonic field* of mass m. The *wave equation* ($m = 0$) is a particular case of the Klein-Gordon equation. Note that since $-\Box + m^2$ preserves real functions, the Klein-Gordon equation has real solutions, which are associated to *neutral fields*, corresponding to neutral particles, while the complex solutions are associated to *charged fields*, corresponding to charged particles.

It will be more convenient later to consider complex solutions, but in this chapter we will, as is usual in the physics literature, consider mainly real solutions. The case of complex solutions will be briefly discussed in Section 2.4.

We refer the reader to Chapter 4 for a general discussion of the real vs complex formalism in a more abstract framework.

We are interested in the space of its *smooth, space-compact, real* solutions denoted by $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$. $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$ is invariant under the Poincaré group if we set

$$\alpha_\Lambda \phi(x) := \phi(\Lambda^{-1} x), \quad \Lambda \in P(1,d). \tag{2.3}$$

2.2.1. The Cauchy problem. If $\phi \in C^\infty(\mathbb{R}^n)$ and $t \in \mathbb{R}$ we set $\phi(t)(\mathrm{x}) := \phi(t,\mathrm{x}) \in C^\infty(\mathbb{R}^d)$. Any solution $\phi \in \mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$ is determined by its Cauchy data on the Cauchy surface $\Sigma_s = \{t = s\} \sim \mathbb{R}^d$, defined by the map

$$\varrho_s\phi := \begin{pmatrix} \phi(s) \\ \partial_t\phi(s) \end{pmatrix} = f \in C_0^\infty(\mathbb{R}^d;\mathbb{R}^2). \tag{2.4}$$

The unique solution in $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$ of the Cauchy problem

$$\begin{cases} (-\Box + m^2)\phi = 0, \\ \varrho_s\phi = f, \end{cases} \tag{2.5}$$

is denoted by $\phi = U_s f$ and given by

$$\phi(t) = \cos(\epsilon(t-s))f_0 + \epsilon^{-1}\sin(\epsilon(t-s)f_1, \quad f = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}. \tag{2.6}$$

The map U_s is called the *Cauchy evolution operator*. The following proposition expresses the important *causality property* of U_s.

PROPOSITION 2.2.1. *One has*

$$\operatorname{supp} U_s f \subset J(\{s\} \times \operatorname{supp} f).$$

2.2.2. Advanced and retarded inverses. Let us now consider the *inhomogeneous Klein-Gordon equation*

$$(-\Box + m^2)u = v, \tag{2.7}$$

where for simplicity $v \in C_0^\infty(\mathbb{R}^n)$. Since there are plenty of homogeneous solutions, it is necessary to supplement (2.7) by *support conditions* to obtain unique solutions, by requiring that ϕ vanishes for large negative or positive times.

THEOREM 2.2.2. (1) *there exist unique solutions* $u_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}}v \in C^{\infty\pm}_{\mathrm{sc}}(\mathbb{R}^n)$ *of* (2.7). *Setting*

$$G_{\mathrm{ret/adv}}(t) := \pm\theta(\pm t)\epsilon^{-1}\sin(\epsilon t), \tag{2.8}$$

where $\theta(t) = \mathbb{1}_{[0,+\infty[}(t)$ *is the Heaviside function, one has*

$$G_{\mathrm{ret/adv}}v(t,\cdot) = \int_{\mathbb{R}} G_{\mathrm{ret/adv}}(t-s)v(s,\cdot)ds; \tag{2.9}$$

(2) *one has* $\operatorname{supp} G_{\mathrm{ret/adv}}v \subset J_\pm(\operatorname{supp} v)$.

The operators $G_{\mathrm{ret/adv}}$ are called the *retarded/advanced inverses* of P. Let us equip $C_0^\infty(\mathbb{R}^n)$ with the scalar product

$$(u|v)_{\mathbb{R}^n} := \int_{\mathbb{R}^n} \overline{u}v dx, \tag{2.10}$$

and $C_0^\infty(\mathbb{R}^d;\mathbb{C}^2)$ with the scalar product

$$(f|g)_{\mathbb{R}^d} = \int_{\mathbb{R}^d} \big(\overline{f}_1 g_1 + \overline{f}_0 g_0\big)d\mathrm{x}. \tag{2.11}$$

It follows from (2.8) that

$$G^*_{\mathrm{ret/adv}} = G_{\mathrm{adv/ret}},$$

where A^* denotes the formal adjoint of A with respect to the scalar product $(\cdot|\cdot)_{\mathbb{R}^n}$. The operator

$$G := G_{\mathrm{ret}} - G_{\mathrm{adv}} \tag{2.12}$$

is called in the physics literature the *Pauli-Jordan* or *commutator function*, or also the *causal propagator*. Note that

$$G = -G^*, \quad \operatorname{supp} Gv \subset J(\operatorname{supp} v), \tag{2.13}$$

and

$$Gv(t,\cdot) = \int_{\mathbb{R}} \epsilon^{-1} \sin(\epsilon(t-s))v(s,\cdot)ds. \tag{2.14}$$

There is an important relationship between G and U_s. Namely, if we denote by $\varrho_s^* : \mathcal{D}'(\mathbb{R}^d;\mathbb{R}^2) \to \mathcal{D}'(\mathbb{R}^n)$ the formal adjoint of $\varrho_s : C_0^\infty(\mathbb{R}^n) \to C_0^\infty(\mathbb{R}^d;\mathbb{R}^2)$ with respect to the scalar products (2.10) and (2.11), then:

$$\varrho_s^* f(t,\mathrm{x}) = \delta_s(t) \otimes f_0(\mathrm{x}) - \delta_s'(t) \otimes f_1(\mathrm{x}), \quad f \in C^\infty(\mathbb{R}^d;\mathbb{R}^2). \tag{2.15}$$

The following lemma follows from (2.6), (2.8) by a direct computation.

LEMMA 2.2.3. *One has*

$$U_s f = G^* \circ \varrho_s^* \circ \sigma f, \quad f \in C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),$$

for $\sigma = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$.

2.2.3. Symplectic structure. It is well-known that the Klein-Gordon equation is a Hamiltonian equation. Indeed let us equip $C_0^\infty(\mathbb{R}^d;\mathbb{R}^2)$ with the symplectic form:

$$f \cdot_\sigma g := \int_{\mathbb{R}^d} \big(f_1 g_0 - f_0 g_1\big) d\mathrm{x}. \tag{2.16}$$

If we identify bilinear forms on $C_0^\infty(\mathbb{R}^d;\mathbb{R}^2)$ with linear operators using the scalar product $(\cdot|\cdot)_{\mathbb{R}^d}$, we have

$$f \cdot_\sigma g = (f|\sigma g)_{\mathbb{R}^d},$$

where the operator σ is defined in Lemma 2.2.3. If we introduce the *classical Hamiltonian*

$$f \cdot E f := \frac{1}{2} \int_{\mathbb{R}^d} \big(f_1^2 + f_0 \epsilon^2 f_0\big) d\mathrm{x}$$

and define $A \in L(C_0^\infty(\mathbb{R}^d;\mathbb{R}^2))$ by

$$f \cdot_\sigma A g := f \cdot E g, \ \ f, g \in C_0^\infty(\mathbb{R}^d;\mathbb{R}^2), \tag{2.17}$$

we obtain that

$$A = \begin{pmatrix} 0 & \mathbb{1} \\ -\epsilon^2 & 0 \end{pmatrix}.$$

Setting $f(t) = \varrho_t U_0 f$ for $f \in C_0^\infty(\mathbb{R}^d;\mathbb{C}^2)$ we have, by an easy computation

$$f(t) = \mathrm{e}^{tA} f, \tag{2.18}$$

which shows that $f \mapsto f(t)$ is the symplectic flow generated by the classical Hamiltonian E and the symplectic form σ. In particular, if $f_i(t) = \mathrm{e}^{tA} f_i$, $i = 1, 2$, $f_1(t) \cdot_\sigma f_2(t)$ is independent on t.

Equivalently, we can equip $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$ with the symplectic form

$$\phi_1 \cdot_\sigma \phi_2 := \varrho_t \phi_1 \cdot_\sigma \varrho_t \phi_2, \tag{2.19}$$

where the right-hand side is independent on t. Fixing the reference Cauchy surface $\Sigma_0 \sim \mathbb{R}^d$, we obtain the following proposition:

PROPOSITION 2.2.4. *The Cauchy data map on* Σ_0

$$\varrho_0 : (\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG), \sigma) \longrightarrow (C_0^\infty(\mathbb{R}^d;\mathbb{R}^2), \sigma),$$

is symplectic, with $\varrho_0^{-1} = U_0$*, where the Cauchy evolution operator* U_s *was introduced in Subsection 2.2.1.*

This leads to another interpretation of (2.18): the space $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$ is invariant under the group of time translations

$$\tau_s\phi(\cdot,\mathrm{x}) := \phi(\cdot - s,\mathrm{x}),$$

and τ_s is symplectic on $(\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG),\sigma)$. Then (2.18) can be rewritten as

$$\varrho_0 \circ \tau_s \circ \varrho_0^{-1} = \mathrm{e}^{sA}, \quad s \in \mathbb{R}.$$

2.3. Pre-symplectic space of test functions

By Proposition 2.2.4, $(\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG),\sigma)$ is a symplectic space. It is easy to see that α_Λ defined in (2.3) is symplectic if Λ is orthochronous, for example using Theorem 2.3.2 below. If Λ is anti-orthochronous, α_Λ is *anti-symplectic*, i.e. transforms σ into $-\sigma$.

Identifying $(\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG),\sigma)$ with $(C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),\sigma)$ using ϱ_0 is convenient for concrete computations, but destroys Poincaré invariance, since one fixes the Cauchy surface Σ_0. It would be useful to have another isomorphic symplectic space which is Poincaré invariant and at the same time easier to understand than $\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$. It turns out that one can use the space of *test functions* $C_0^\infty(\mathbb{R}^n;\mathbb{R})$, which is a fundamental step in formulating the notion of *locality* for quantum fields.

Proposition 2.3.1. *Consider the map $G : C_0^\infty(\mathbb{R}^n;\mathbb{R}) \to C_{\mathrm{sc}}^\infty(\mathbb{R}^n)$. Then:*

(1) $\mathrm{Ran}G = \mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$,

(2) $\mathrm{Ker}\, G = PC_0^\infty(\mathbb{R}^n;\mathbb{R})$.

Moreover, we have

(3) $(\varrho_0 G)^* \circ \sigma \circ (\varrho_0 G) = G$.

Proof. (1) By $P \circ G = 0$ and Theorem 2.2.2 (2), we see that $\mathrm{Ran}G \subset \mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$. Conversely let $\phi \in \mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG)$. If $f_s = \varrho_s\phi$, then by Lemma 2.2.3 we obtain that $\phi = -G \circ \varrho_s^* \circ \sigma f_s$ for $s \in \mathbb{R}$. Hence, if $\chi \in C_0^\infty(\mathbb{R})$ with $\int \chi(s)ds = 1$ we obtain that

$$\phi = \int_{\mathbb{R}} \chi(s)\phi dx = Gv,$$

for $v = -\int_{\mathbb{R}} \varrho_s^* \circ \sigma f_s ds \in C_0^\infty(\mathbb{R}^n)$.

(2) Since $G \circ P = 0$ we have $PC_0^\infty(\mathbb{R}^n;\mathbb{R}) \subset \mathrm{Ker}\, G$. Conversely let $v \in C_0^\infty(\mathbb{R}^n;\mathbb{R})$ with $Gv = 0$. Then for $u_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}}v$ we have $u_{\mathrm{ret}} = u_{\mathrm{adv}} =: u$, $u \in C_0^\infty(\mathbb{R}^n)$ by Theorem 2.2.2 (2) and $v = Pu$ since $P \circ G_{\mathrm{ret/adv}} = \mathbb{1}$.

(3) We have, using (2.14)

$$\varrho_0 Gu = \begin{pmatrix} -\int \epsilon^{-1}\sin(\epsilon s)u(s)ds \\ \int \cos(\epsilon s)u(s)ds \end{pmatrix},$$

hence

$$\sigma \circ (\varrho_0 G)u = -\begin{pmatrix} \int \cos(\epsilon s)u(s)ds \\ \int \epsilon^{-1}\sin(\epsilon s)u(s)ds \end{pmatrix},$$

and

$$\begin{aligned}(\varrho_0 G)^* f &= -G\varrho_0^* f \\ &= -\int \epsilon^{-1}\sin(\epsilon(t-s))(\delta_0(s)\otimes f_0 - \delta_0'(s)\otimes f_1)ds \\ &= -\epsilon^{-1}\sin(\epsilon t)f_0 + \cos(\epsilon t)f_1,\end{aligned}$$

which yields

$$\begin{aligned}&(\varrho_0 G)^* \circ \sigma \circ (\varrho_0 G)u \\ &\quad = \int \epsilon^{-1}\sin(\epsilon t)\cos(\epsilon s)u(s)ds + \int \epsilon^{-1}\cos(\epsilon t)\sin(\epsilon s)u(s)ds \\ &\quad = \int \epsilon^{-1}\sin(\epsilon(t-s))u(s)ds = Gu.\end{aligned}$$

This completes the proof of the proposition. □

One can summarize Propositions 2.2.4 and 2.3.1 in the following theorem:

THEOREM 2.3.2. (1) *The following spaces are symplectic spaces:*

$$(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{R})}{PC_0^\infty(\mathbb{R}^n;\mathbb{R})},(\cdot|G\cdot)_{\mathbb{R}^n}),\quad (\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG),\sigma),\quad (C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),\sigma).$$

(2) *The following maps are symplectomorphisms:*

$$(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{R})}{PC_0^\infty(\mathbb{R}^n;\mathbb{R})},(\cdot|G\cdot)_{\mathbb{R}^n}) \xrightarrow{G} (\mathrm{Sol}_{\mathrm{sc},\mathbb{R}}(KG),\sigma) \xrightarrow{\varrho_0} (C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),\sigma).$$

The first and last of these equivalent symplectic spaces are the most useful for the quantization of the Klein-Gordon equation.

2.4. The complex case

Let us now discuss the space $\mathrm{Sol}_{\mathrm{sc},\mathbb{C}}(KG)$ of *complex* space-compact solutions. We refer to Section 4.2 for notation and terminology.

It is more natural to use the map

$$\varrho_s\phi := \begin{pmatrix} \phi(s) \\ \mathrm{i}^{-1}\partial_t\phi(s) \end{pmatrix} \tag{2.20}$$

as Cauchy data map and to equip the space $C_0^\infty(\mathbb{R}^d;\mathbb{C}^2)$ of Cauchy data with the Hermitian form

$$\overline{f}\cdot qg := \int_{\mathbb{R}^d} \big(\overline{f}_1 g_0 + \overline{f_0} g_1\big) d\mathrm{x}. \tag{2.21}$$

The space $\mathrm{Sol}_{\mathrm{sc},\mathbb{C}}(KG)$ is similarly equipped with the form

$$\overline{\phi}_1\cdot q\phi_2 := \overline{\varrho_t\phi}_1\cdot q\varrho_t\phi_2,$$

which is independent on t. The Cauchy evolution operator becomes

$$U_0 f(t) = \cos(\epsilon t) f_0 + \mathrm{i}\epsilon^{-1}\sin(\epsilon t) f_1. \tag{2.22}$$

We have then the following analog of Theorem 2.3.2:

THEOREM 2.4.1. (1) *The following spaces are Hermitian spaces:*

$$(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{C})}{PC_0^\infty(\mathbb{R}^n;\mathbb{C})},(\cdot|\mathrm{i}G\cdot)_{\mathbb{R}^n}),\quad (\mathrm{Sol}_{\mathrm{sc},\mathbb{C}}(KG),q),\quad (C_0^\infty(\mathbb{R}^d;\mathbb{C}^2),q).$$

(2) *The following maps are unitary:*

$$(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{C})}{PC_0^\infty(\mathbb{R}^n;\mathbb{C})},(\cdot|\mathrm{i}G\cdot)_{\mathbb{R}^n}) \xrightarrow{G} (\mathrm{Sol}_{\mathrm{sc},\mathbb{C}}(KG),q) \xrightarrow{\varrho_0} (C_0^\infty(\mathbb{R}^d;\mathbb{C}^2),q).$$

CHAPTER 3

Fock quantization on Minkowski space

We describe in this chapter the *Fock quantization* of the Klein-Gordon equation on Minkowski spacetime. We recall the definition of the *bosonic Fock space* over a one-particle space and of the *creation/annihilation operators*, which are ubiquitous notions in quantum field theory.

For example, it is common in the physics oriented literature to specify a state for the Klein-Gordon field by defining first some creation/annihilation operators. We will see in Chapter 4 that this is nothing else than choosing a particular Kähler structure on a certain symplectic space.

In this approach the quantum Klein-Gordon fields are defined as linear operators on the Fock space, so one has to pay attention to domain questions. These technical problems disappear if one uses a more abstract point of view and introduces the appropriate CCR $*$-*algebra*, as will be done in Chapter 4. Fock spaces will reappear as the (Gelfand-Naimark-Segal) GNS *Hilbert spaces* associated to a pure quasi-free state on this algebra. Apart from this fact, they can be forgotten.

3.1. Bosonic Fock space

3.1.1. Bosonic Fock space. Let $\mathfrak{h}$ be a complex Hilbert space whose unit vectors describe the states of a quantum particle. If this particle is *bosonic*, then the states of a system of n such particles are described by unit vectors in the *symmetric tensor power* $\otimes_{\mathrm{s}}^n\mathfrak{h}$, where we take the tensor products in the Hilbert space sense, i.e. complete the algebraic tensor products for the natural Hilbert norm.

A system of an arbitrary number of particles is described by the *bosonic Fock space*

$$\Gamma_{\mathrm{s}}(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \otimes_{\mathrm{s}}^n \mathfrak{h}, \tag{3.1}$$

where the direct sum is again taken in the Hilbert space sense and $\otimes_{\mathrm{s}}^0\mathfrak{h} = \mathbb{C}$ by definition. We recall that the symmetrized tensor product is defined by

$$\Psi_1 \otimes_{\mathrm{s}} \Psi_2 := \Theta_{\mathrm{s}}(\Psi_1 \otimes \Psi_2),$$

where

$$\Theta_{\mathrm{s}}(u_1 \otimes \cdots \otimes u_n) = \frac{1}{n!} \sum_{\sigma \in S_n} u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)}.$$

The vector $\Omega_{\mathrm{vac}} = (1, 0, \dots)$ is called the *vacuum* and describe a state with no particles at all. A useful observable on $\Gamma_{\mathrm{s}}(\mathfrak{h})$ is the *number operator* N, which counts the number of particles, defined by

$$N|_{\otimes_{\mathrm{s}}^n \mathfrak{h}} = n\mathbb{1}.$$

The operator N is an example of a *second quantized operator*, namely $N = \mathrm{d}\Gamma(\mathbb{1})$, where

$$d\Gamma(a)|_{\otimes_{\mathrm{s}}^n \mathfrak{h}} := \sum_{j=1}^{n} \mathbb{1}^{\otimes j-1} \otimes a \otimes \mathbb{1}^{\otimes n-j},$$

for a a linear operator on $\mathfrak{h}$.

3.1.2. Creation/annihilation operators. Since $\Gamma_{\rm s}(\mathfrak{h})$ describes an arbitrary number of particles, it is useful to have operators that create or annihilate particles. One defines the *creation/annihilation operators* by

$$\begin{aligned} a^*(h)\Psi_n &:= \sqrt{n+1}h \otimes_{\rm s} \Psi_n, \\ a(h)\Psi_n &:= \sqrt{n}(h| \otimes \mathbb{1}^{\otimes n-1}\Psi_n, \quad \Psi_n \in \otimes^n_{\rm s}(\mathfrak{h}),\ h \in \mathfrak{h}, \end{aligned}$$

where one sets $(h|u = (h|u)$ for $u \in \mathfrak{h}$. It is easy to see that $a^{(*)}(h)$ are well defined on $\mathrm{Dom}\, N^{\frac{1}{2}}$ and that $(\Psi_1|a^*(h)\Psi_2) = (a(h)\Psi_1|\Psi_2)$, i.e. $a(h)^* \subset a^*(h)$ on $\mathrm{Dom}\, N^{\frac{1}{2}}$. Moreover

$$\mathfrak{h} \ni h \mapsto a^*(h),\ \text{resp. } a(h) \text{ is } \mathbb{C}\text{-linear, resp. anti-linear,} \tag{3.2}$$

and as quadratic forms on $\mathrm{Dom}\, N^{\frac{1}{2}}$ one has

$$\begin{aligned} &[a(h_1), a(h_2)] = [a^*(h_1), a^*(h_2)] = 0, \\ &[a(h_1), a^*(h_2)] = (h_1|h_2)\mathbb{1}, \quad h_1, h_2 \in \mathfrak{h}, \end{aligned} \tag{3.3}$$

where $[A, B] = AB - BA$, which a version of the *canonical commutation relations*, abbreviated CCR in the sequel.

3.1.3. Field and Weyl operators. One then introduces the *field operators* in the Fock representation

$$\phi_{\rm F}(h) := \frac{1}{\sqrt{2}}(a(h) + a^*(h)), \quad h \in \mathfrak{h}, \tag{3.4}$$

which can be easily shown to be essentially selfadjoint on $\mathrm{Dom}\, N^{\frac{1}{2}}$. One has

$$\phi_{\rm F}(h_1 + \lambda h_2) = \phi_{\rm F}(h_1) + \lambda\phi_{\rm F}(h_2), \quad \lambda \in \mathbb{R}, h_i \in \mathfrak{h},\ \text{on } \mathrm{Dom}\, N^{\frac{1}{2}}, \tag{3.5}$$

i.e. $h \longmapsto \phi_{\rm F}(h)$ is $\mathbb{R}$-linear, and the *Heisenberg form* of the CCR are satisfied as quadratic forms on $\mathrm{Dom}\, N^{\frac{1}{2}}$

$$[\phi_{\rm F}(h_1), \phi_{\rm F}(h_2)] = {\rm i}h_1 \cdot \sigma h_2 \mathbb{1}. \tag{3.6}$$

for

$$h_1 \cdot \sigma h_2 = \mathrm{Im}(h_1|h_2). \tag{3.7}$$

Denoting again by $\phi_{\rm F}(h)$ the selfadjoint closure of $\phi_{\rm F}(h)$, one can then define the *Weyl operators*

$$W_{\rm F}(h) := {\rm e}^{{\rm i}\phi_{\rm F}(h)}, \tag{3.8}$$

which are unitary and satisfy the *Weyl form* of the CCR

$$W_{\rm F}(h_1)W_{\rm F}(h_2) = {\rm e}^{-{\rm i}h_1 \cdot \sigma h_2} W_{\rm F}(h_1 + h_2).$$

If $\mathfrak{h}_{\mathbb{R}}$ denotes the real form of $\mathfrak{h}$, i.e. $\mathfrak{h}$ as a real vector space, then $(\mathfrak{h}_{\mathbb{R}}, \sigma)$ is a real symplectic space. Moreover i, considered as an element of $L(\mathfrak{h}_{\mathbb{R}})$, belongs to $Sp(\mathfrak{h}_{\mathbb{R}}, \sigma)$ and one has

$$\nu := \sigma \circ {\rm i} = \mathrm{Re}(\cdot|\cdot) \geq 0.$$

3.1.4. Kähler structures. In general, a triple $(\mathcal{X}, \sigma, \mathrm{j})$, where $(\mathcal{X}, \sigma)$ is a real symplectic space and $\mathrm{j} \in L(\mathcal{X})$ satisfies $\mathrm{j}^2 = -\mathbb{1}$ and $\sigma \circ \mathrm{j} \in L_{\mathrm{s}}(\mathcal{X}, \mathcal{X}')$, is called a *pseudo-Kähler structure* on $\mathcal{X}$. If $\sigma \circ \mathrm{j} \geq 0$, it is called a *Kähler structure*. The anti-involution j is called a *Kähler anti-involution*. We will come back to this notion in Section 4.1. Given a Kähler structure on $\mathcal{X}$, one can turn $\mathcal{X}$ into a complex pre-Hilbert space by equipping it with the complex structure j and the scalar product:

$$(x_1|x_2)_{\mathrm{F}} := x_1 \cdot \sigma \mathrm{j} x_2 + \mathrm{i} x_1 \cdot \sigma x_2. \tag{3.9}$$

If we choose as one-particle Hilbert space the completion of $\mathcal{X}$ for $(\cdot|\cdot)_{\mathrm{F}}$, we can construct the *Fock representation* by the map

$$\mathcal{X} \ni x \longmapsto \phi_{\mathrm{F}}(x)$$

which satisfies (3.5), (3.6).

3.2. Fock quantization of the Klein-Gordon equation

From the above discussion we see that the first step in the construction of quantum Klein-Gordon fields is to fix a Kähler anti-involution on one of the equivalent symplectic spaces in Theorem 2.3.2, the most convenient one being $(C_0^\infty(\mathbb{R}^d; \mathbb{R}^2), \sigma)$.

3.2.1. The Kähler structure. There are plenty of choices of Kähler anti-involutions. The most natural one is obtained as follows: let us denote by $\mathfrak{h}$ the completion of $C_0^\infty(\mathbb{R}^d; \mathbb{C})$ with respect to the scalar product

$$(h_1|h_2)_{\mathrm{F}} := (h_1|\epsilon^{-1} h_2)_{\mathbb{R}^d}.$$

If $m > 0$, this space is the (complex) Sobolev space $H^{-\frac{1}{2}}(\mathbb{R}^d)$ and if $m = 0$ the complex homogeneous Sobolev space $\dot{H}^{-\frac{1}{2}}(\mathbb{R}^d)$, except when $d = 1$, since the integral $\int_{\mathbb{R}} |\mathrm{k}|^{-1} d\mathrm{k}$ diverges at $\mathrm{k} = 0$. This is an example of the so-called *infrared problem* for massless fields in two spacetime dimensions.

To avoid a somewhat lengthy digression, we will assume that $m > 0$ if $d = 1$. Let us introduce the map

$$V : C_0^\infty(\mathbb{R}^d; \mathbb{R}^2) \ni f \longmapsto \epsilon f_0 - \mathrm{i} f_1 \in \mathfrak{h}. \tag{3.10}$$

An easy computation shows that:

$$\begin{aligned} &\mathrm{Im}(Vf|Vg)_{\mathrm{F}} = f \cdot \sigma g, \\ &\mathrm{i} \circ V =: V \circ \mathrm{j}, \quad \text{for } \mathrm{j} = \begin{pmatrix} 0 & \epsilon^{-1} \\ -\epsilon & 0 \end{pmatrix}, \\ &\mathrm{e}^{\mathrm{i}t\epsilon} \circ V = V \circ \mathrm{e}^{tA}. \end{aligned}$$

In other words, j is a Kähler anti-involution on $C_0^\infty(\mathbb{R}^d; \mathbb{R}^2)$ and the associated one-particle Hilbert space is unitarily equivalent to $\mathfrak{h}$. Moreover, after identification by V, the symplectic group $\{\mathrm{e}^{tA}\}_{t \in \mathbb{R}}$ becomes the unitary group $\{\mathrm{e}^{\mathrm{i}t\epsilon}\}_{t \in \mathbb{R}}$ with *positive* generator ϵ. This positivity is the distinctive feature of the Fock representation.

3.3. Quantum spacetime fields

Let us set

$$\Phi_{\mathrm{F}}(u) = \int_{\mathbb{R}} \phi_{\mathrm{F}}(\mathrm{e}^{-\mathrm{i}t\epsilon} u(t, \cdot)) dt, \ u \in C_0^\infty(\mathbb{R}^n; \mathbb{R}), \tag{3.11}$$

the integral being for example norm convergent in $B(\mathrm{Dom}\, N^{\frac{1}{2}}, \Gamma_{\mathrm{s}}(\mathfrak{h}))$. We obtain from (2.14) and (3.7) that

$$[\Phi_{\mathrm{F}}(u), \Phi_{\mathrm{F}}(v)] = \mathrm{i}(u|Gv)_{\mathbb{R}^n} \mathbb{1}, \tag{3.12}$$

and $\Phi_{\rm F}(Pu)=0$. Setting formally

$$\Phi_{\rm F}(u) =: \int_{\mathbb{R}^n} \Phi_{\rm F}(x)u(x)dx,$$

we obtain the *spacetime fields* $\Phi_{\rm F}(x)$, which satisfy

$$\begin{aligned} &[\Phi_{\rm F}(x),\Phi_{\rm F}(x')] = {\rm i}G(x-x')\mathbb{1}, \quad x,x'\in\mathbb{R}^n,\\ &(-\Box+m^2)\Phi_{\rm F}(x)=0. \end{aligned} \tag{3.13}$$

3.3.1. The vacuum state. Let us denote by $\mathrm{CCR}^{\rm pol}(KG)$ the $*$-algebra generated by the $\Phi_{\rm F}(u)$, $u\in C_0^\infty(\mathbb{R}^n;\mathbb{R})$, see Subsections 4.3.1 and 4.5.1 below for a precise definition. The vacuum vector $\Omega_{\rm vac}\in\Gamma_{\rm s}(\mathfrak{h})$ induces a *state* $\omega_{\rm vac}$ on $\mathrm{CCR}^{\rm pol}(KG)$, called the *Fock vacuum state*, by

$$\omega_{\rm vac}(\prod_{i=1}^N \Phi_{\rm F}(u_i)) := (\Omega_{\rm vac}|\prod_{i=1}^N \Phi_{\rm F}(u_i)\Omega_{\rm vac})_{\Gamma_{\rm s}(\mathfrak{h})}$$

Clearly, $\omega_{\rm vac}$ induces linear maps

$$\otimes^n C_0^\infty(\mathbb{R}^n;\mathbb{R}) \ni u_1\otimes\cdots\otimes u_N \longmapsto \omega_{\rm vac}(\prod_{i=1}^N \Phi_{\rm F}(u_i))\in\mathbb{C},$$

which are continuous for the topology of $C_0^\infty(\mathbb{R}^n;\mathbb{R})$, and hence one can write

$$\omega_{\rm vac}(\prod_{i=1}^N \Phi_{\rm F}(u_i)) =: \int_{\mathbb{R}^{Nn}} \omega_N(x_1,\ldots,x_N)\prod_{i=1}^N u_i(x_i)dx_1\ldots dx_N,$$

where the distributions $\omega_N\in\mathcal{D}'(\mathbb{R}^{Nn})$ are called in physics the *N-point functions*. Among them the most important one is the 2-*point function* ω_2, which equals

$$\omega_2(x,x') = (2\pi)^{-n}\int_{\mathbb{R}^d}\frac{1}{2\epsilon(\mathrm{k})}{\rm e}^{{\rm i}(t-t')\epsilon(\mathrm{k})+{\rm i}\mathrm{k}\cdot(\mathrm{x}-\mathrm{x}')}d\mathrm{k}. \tag{3.14}$$

If we write similarly the distributional kernel of G, we obtain by (2.14)

$$G(x,x') = (2\pi)^{-n}\int_{\mathbb{R}^d}\frac{1}{\epsilon(\mathrm{k})}\sin((t-t')\epsilon(\mathrm{k})){\rm e}^{{\rm i}\mathrm{k}\cdot(\mathrm{x}-\mathrm{x}')}d\mathrm{k}. \tag{3.15}$$

The fact that $\omega_2(x,x')$ and $G(x-x')$ depend only on $x-x'$ reflects the invariance of the vacuum state $\omega_{\rm vac}$ under space and time translations.

3.4. Local algebras

We recall that a *double cone* is a subset

$$O = I_+(\{x_1\})\cap I_-(\{x_2\}), \quad x_1,x_2\in\mathbb{R}^n \text{ with } x_2\in J_+(x_1).$$

We denote by $\mathfrak{A}(O)$ the norm closure of $\mathrm{Vect}(\{{\rm e}^{{\rm i}\Phi_{\rm F}(u)} : \mathrm{supp}\, u\subset O\})$ in $B(\Gamma_{\rm s}(\mathfrak{h}))$. From (2.13) and (3.12) it follows that

$$[\mathfrak{A}(O_1),\mathfrak{A}(O_2)] = \{0\}, \text{ if } O_1,O_2 \text{ are causally disjoint.}$$

We obtain a representation of the Poincaré group $P(1,d)$ by $*$-automorphisms of $\mathrm{CCR}^{\rm pol}(KG)$ by setting $\alpha_\Lambda\Phi_{\rm F}(x)=\Phi_{\rm F}(\Lambda^{-1}x)$ for $\Lambda\in P(1,d)$. From the invariance of the vacuum state under translations, we obtain that $\alpha_{(a,\mathbb{1})}(A)=U(a)AU(a)^{-1}$ for $A\in\mathrm{CCR}^{\rm pol}(KG)$, where $\mathbb{R}^n\ni a\mapsto U(a)$ is a strongly continuous unitary group on $\Gamma_{\rm s}(\mathfrak{h})$.

We have $\alpha_\Lambda(\mathfrak{A}(O))=\mathfrak{A}(LO+a)$, for $\Lambda=(a,L)\in P(1,d)$.

3.4.1. The Reeh-Schlieder property. One might expect that the closed subspace generated by the vectors $A\Omega_{\rm vac}$ for $A \in \mathfrak{A}(O)$ depends on O, since it describes excitations of the vacuum $\Omega_{\rm vac}$ localized in O. This is not the case, and actually the following *Reeh-Schlieder* property holds:

PROPOSITION 3.4.1. *For any double cone O the space $\{A\Omega_{\rm vac} : A \in \mathfrak{A}(O)\}$ is dense in $\Gamma_{\rm s}(\mathfrak{h})$.*

Proof. Let $u \in \Gamma_{\rm s}(\mathfrak{h})$ such that $(u|A\Omega_{\rm vac}) = 0$ for all $A \in \mathfrak{A}(O)$. If $O_1 \Subset O$ is a smaller double cone and $A \in \mathfrak{A}(O_1)$, the function $f : \mathbb{R}^n \ni x \mapsto (u|U(x)A\Omega_{\rm vac})$ has a holomorphic extension F to $\mathbb{R}^n + {\rm i}C_+$, i.e. $f(x) = F(x + {\rm i}C_+ 0)$, as distributional boundary values, see Section 12.1.

Since $U(x)AU^*(x) \in \mathfrak{A}(O)$, we have $f(x) = 0$ for x close to 0, hence by the edge of the wedge theorem, see Subsection 12.1.2, $F = 0$ and $f = 0$ on $\mathbb{R}^n$. Vectors of the form $U(x)A\Omega_{\rm vac}$ for $x \in \mathbb{R}^n, A \in \mathfrak{A}(O_1)$ are dense in $\Gamma_{\rm s}(\mathfrak{h})$, hence $u = 0$. □

CHAPTER 4

CCR algebras and quasi-free states

In this chapter we collect various well-known results on the CCR $*$-algebras associated to a symplectic space and on *quasi-free states*. We will often work with *complex* symplectic spaces, which will be convenient later on when one considers Klein-Gordon fields. We follow the presentation in [**DG**, Section 17.1] and [**GW1**, Section 2].

4.1. Vector spaces

In this subsection we collect some useful notation, following [**DG**, Section 1.2].

4.1.1. Real vector spaces. Real vector spaces will be usually denoted by $\mathcal{X}$. The complexification of a real vector space $\mathcal{X}$ will be denoted by $\mathbb{C}\mathcal{X} = \{x_1 + \mathrm{i}x_2 : x_1, x_2 \in \mathcal{X}\}$.

4.1.2. Complex vector spaces. Complex vector spaces will be usually denoted by $\mathcal{Y}$. If $\mathcal{Y}$ is a complex vector space, its *real form*, i.e. $\mathcal{Y}$, regarded as a vector space over $\mathbb{R}$, will be denoted by $\mathcal{Y}_{\mathbb{R}}$.

Conversely, a real vector space $\mathcal{X}$ equipped with an *anti-involution* j (also called a *complex structure*), i.e. $\mathrm{j} \in L(\mathcal{X})$ with $\mathrm{j}^2 = -\mathbb{1}$ can be equipped with the structure of a complex space by setting

$$(\lambda + \mathrm{i}\mu)x = \lambda x + \mu \mathrm{j}x, \quad x \in \mathcal{X},\ \lambda + \mathrm{i}\mu \in \mathbb{C}.$$

If $\mathcal{Y}$ is a complex vector space, we denote by $\overline{\mathcal{Y}}$ the *conjugate vector space* of $\mathcal{Y}$, i.e. $\overline{\mathcal{Y}} = \mathcal{Y}_{\mathbb{R}}$ as a real vector space, equipped with the complex structure $-\mathrm{j}$, if $\mathrm{j} \in L(\mathcal{Y}_{\mathbb{R}})$ is the complex structure of $\mathcal{Y}$. The identity map $\mathbb{1} : \mathcal{Y} \to \overline{\mathcal{Y}}$ will be denoted by $y \mapsto \overline{y}$, i.e. $\overline{y}$ equals y, but considered as an element of $\overline{\mathcal{Y}}$. The map $\mathbb{1} : \mathcal{Y} \to \overline{\mathcal{Y}}$ is anti-linear.

4.1.3. Duals and antiduals. Let $\mathcal{X}$ be a real vector space. Its dual will be denoted by $\mathcal{X}'$.

Let $\mathcal{Y}$ be a complex vector space. Its dual will be denoted by $\mathcal{Y}'$, and its anti-dual, i.e. the space of $\mathbb{C}$-anti-linear forms on $\mathcal{Y}$, by $\mathcal{Y}^*$. By definition, $\mathcal{Y}^* = \overline{\mathcal{Y}}'$. Note that we have a $\mathbb{C}$-linear identification $\overline{\mathcal{Y}'} \sim \overline{\mathcal{Y}}'$ defined as follows: if $y \in \mathcal{Y}$ and $w \in \mathcal{Y}'$, then

$$\overline{w} \cdot \overline{y} := \overline{w \cdot y}.$$

This identifies $\overline{w} \in \overline{\mathcal{Y}'}$ with an element of $\overline{\mathcal{Y}}'$. Similarly, we have a $\mathbb{C}$-linear identification $\overline{\mathcal{Y}}^* \sim \overline{\mathcal{Y}^*}$.

4.1.4. Linear operators. If $\mathcal{X}_i$, $i = 1, 2$, are real or complex vector spaces and $a \in L(\mathcal{X}_1, \mathcal{X}_2)$, we denote by $a' \in L(\mathcal{X}_2', \mathcal{X}_1')$ or ${}^t a$ its transpose. If $\mathcal{Y}_i$, $i = 1, 2$ are complex vector spaces we denote by $a^* \in L(\mathcal{Y}_2^*, \mathcal{Y}_1^*)$ its adjoint, and by $\overline{a} \in L(\overline{\mathcal{Y}}_1, \overline{\mathcal{Y}}_2)$ its *conjugate*, defined by $\overline{a}\,\overline{y}_1 = \overline{a y_1}$. With the above identifications we have $a^* = \overline{a}' = \overline{a'}$. If $\mathcal{X}_i$, $i = 1, 2$ are real vector spaces and $a \in L(\mathcal{X}_1, \mathcal{X}_2)$, we denote by $a_{\mathbb{C}} \in L(\mathbb{C}\mathcal{X}_1, \mathbb{C}\mathcal{X}_2)$ its complexification.

4.2. Bilinear and sesquilinear forms

If $\mathcal{X}$ is a real or complex vector space, a bilinear form on $\mathcal{X}$ is given by an operator $a \in L(\mathcal{X}, \mathcal{X}')$, its action on a couple (x_1, x_2) is denoted by $x_1 \cdot a x_2$. We denote by $L_{\mathrm{s/a}}(\mathcal{X}, \mathcal{X}')$ the symmetric/antisymmetric forms on $\mathcal{X}$. A form a is *non-degenerate* if $\operatorname{Ker} a = \{0\}$.

Similarly, if $\mathcal{Y}$ is a complex vector space, a sesquilinear form on $\mathcal{Y}$ is given by an operator $a \in L(\mathcal{Y}, \mathcal{Y}^*)$, and its action on a couple (y_1, y_2) will be denoted by

$$(y_1|ay_2) \quad \text{or} \quad \overline{y}_1 \cdot a y_2, \tag{4.1}$$

the last notation being a reminder that $\mathcal{Y}^* \sim \overline{\mathcal{Y}}'$. We denote by $L_{\mathrm{h/a}}(\mathcal{Y}, \mathcal{Y}^*)$ the Hermitian/anti-Hermitian forms on $\mathcal{Y}$. Non-degenerate forms are defined as in the real case.

If $\mathcal{X}$ is a real vector space and $a \in L(\mathcal{X}, \mathcal{X}')$, we denote by $a_{\mathbb{C}} \in L(\mathbb{C}\mathcal{X}, \mathbb{C}\mathcal{X}^*)$ its *sesquilinear* extension.

4.2.1. Real symplectic spaces. An antisymmetric form $\sigma \in L(\mathcal{X}, \mathcal{X}')$ is called a *pre-symplectic form*. A non-degenerate pre-symplectic form is called *symplectic* and a couple $(\mathcal{X}, \sigma)$ where σ is (pre) symplectic a (real) (*pre*) *symplectic space*.

If $(\mathcal{X}, \sigma)$ is symplectic, the *symplectic group* $Sp(\mathcal{X}, \sigma)$ is the set of invertible $r \in L(\mathcal{X})$ such that $r'\sigma r = \sigma$ equipped with the usual product. The Lie algebra $sp(\mathcal{X}, \sigma)$ is the set of $a \in L(\mathcal{X})$ such that $a'\sigma = -\sigma a$, equipped with the commutator.

4.2.2. Pseudo-Euclidean spaces. A pair $(\mathcal{X}, \nu)$ with $\nu \in L(\mathcal{X}, \mathcal{X}')$ non-degenerate and symmetric is called a *pseudo-Euclidean space*. If $\nu > 0$, it is called an *Euclidean space*. The *orthogonal group* $O(\mathcal{X}, \nu)$ is the set of invertible $r \in L(\mathcal{X})$ such that $r'\nu r = \nu$, equipped with the usual product. The Lie algebra $o(\mathcal{X}, \nu)$ is the set of $a \in L(\mathcal{X})$ such that $a'\nu = -\nu a$, equipped with the commutator.

4.2.3. Hermitian spaces. A space $(\mathcal{Y}, q)$ with q Hermitian is called a *pre-Hermitian space*. If q is non-degenerate, $(\mathcal{Y}, q)$ is called a *Hermitian space*. If $q > 0$ it is called a *pre-Hilbert space*.

The (*pseudo*)*-unitary group* $U(\mathcal{Y}, q)$ is the set of invertible $u \in L(\mathcal{Y})$ such that $u^* q u = q$ equipped with the usual product.

4.2.4. Complex symplectic spaces. An anti-Hermitian form σ on $\mathcal{Y}$ is called a (complex) *pre-symplectic form*. One sets then $q := \mathrm{i}\sigma \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$ called the *charge*. One identifies in this way complex (pre-)symplectic spaces with (pre-)Hermitian spaces. The complex structure on $\mathcal{Y}$ is sometimes called the *charge complex structure* and will often be denoted by j to avoid confusion with the imaginary unit $\mathrm{i} \in \mathbb{C}$.

4.2.5. Charge reversal.

Definition 4.2.1. *Let $(\mathcal{Y}, q)$ a pre-Hermitian space. A map $\chi \in L(\mathcal{Y}_{\mathbb{R}})$ is called a* charge reversal *if $\chi^2 = \mathbb{1}$ or $\chi^2 = -\mathbb{1}$ and*

$$\overline{\chi y}_1 \cdot q \chi y_2 = -\overline{y}_2 \cdot q y_1 \quad y_1, y_2 \in \mathcal{Y}.$$

Note that a charge reversal is anti-linear.

4.2.6. Pseudo-Kähler structures. Let $(\mathcal{Y}, q)$ be a Hermitian space whose complex structure is denoted by $\mathrm{j} \in L(\mathcal{Y}_{\mathbb{R}})$. Note that $(\mathcal{Y}_{\mathbb{R}}, \mathrm{Im}q)$ is a real symplectic space with $\mathrm{j} \in Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Im}q)$ and $\mathrm{j}^2 = -\mathbb{1}$. The converse construction is as follows: a real symplectic space $(\mathcal{X}, \sigma)$ with a map $\mathrm{j} \in L(\mathcal{X})$ such that

$$\mathrm{j}^2 = -\mathbb{1},\ \mathrm{j} \in Sp(\mathcal{X}, \sigma),$$

is called a *pseudo-Kähler space*. If in addition $\nu := \sigma\mathrm{j}$ is positive definite, it is called a *Kähler space*. We set now

$$\mathcal{Y} = (\mathcal{X}, \mathrm{j}),$$

which is a complex vector space, whose elements are logically denoted by y. If $(\mathcal{X}, \sigma, \mathrm{j})$ is a pseudo-Kähler space we can set

$$\overline{y}_1 q y_2 := y_1 \cdot \sigma \mathrm{j} y_2 + \mathrm{i} y_1 \cdot \sigma y_2, \quad y_1, y_2 \in \mathcal{Y},$$

and check that $q \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$ is non-degenerate.

4.3. Algebras

A unital algebra over $\mathbb{C}$ equipped with an anti-linear involution $A \mapsto A^*$ such that $(AB)^* = B^*A^*$ is called a $*$-*algebra*. A $*$-algebra which is complete for a norm such that $\|A\| = \|A^*\|$ and $\|AB\| \leq \|A\|\|B\|$ is called a *Banach* $*$-*algebra*. If moreover $\|A^*A\| = \|A\|^2$, it is called a C^*-*algebra*.

4.3.1. Algebras defined by generators and relations. In physics many algebras are defined by specifying a set of generators and the relations they satisfy. Let us recall the corresponding rigorous definition.

Let $\mathcal{A}$ be a set, called the set of *generators*, and $C_{\mathrm{c}}(\mathcal{A}; \mathbb{K})$ be the vector space of functions $\mathcal{A} \to \mathbb{K}$ with finite support (usually $\mathbb{K} = \mathbb{C}$). Denoting the indicator function $\mathbb{1}_{\{a\}}$ simply by a, we see that every element of $C_{\mathrm{c}}(\mathcal{A}; \mathbb{K})$ can be written as $\sum_{a \in \mathcal{B}} \lambda_a a$, with $\mathcal{B} \subset \mathcal{A}$ finite, $\lambda_a \in \mathbb{K}$.

Thus $C_{\mathrm{c}}(\mathcal{A}; \mathbb{K})$ can be seen as the vector space of finite linear combinations of elements of $\mathcal{A}$. We set

$$\mathfrak{A}(\mathcal{A}, \mathbb{K}) := \otimes C_{\mathrm{c}}(\mathcal{A}; \mathbb{K}),$$

where $\otimes E$ is the tensor algebra over the $\mathbb{K}$-vector space E. Usually one writes $a_1 \cdots a_n$ instead of $a_1 \otimes \cdots \otimes a_n$ for $a_i \in \mathcal{A}$.

Let now $\mathfrak{R} \subset \mathfrak{A}(\mathcal{A}, \mathbb{K})$ (the set of 'relations'). We denote by $\mathfrak{I}(\mathfrak{R})$ the two-sided ideal of $\mathfrak{A}(\mathcal{A}; \mathbb{K})$ generated by $\mathfrak{R}$. Then the quotient

$$\mathfrak{A}(\mathcal{A}, \mathbb{K})/\mathfrak{I}(\mathfrak{R})$$

is called the *unital algebra with generators* $\mathcal{A}$ *and relations* $R = 0, \quad R \in \mathfrak{R}$.

4.3.2. $*$-algebras defined by generators and relations. Assume that $\mathbb{K} = \mathbb{C}$ and let $i : \mathcal{A} \to \mathcal{A}$ some fixed involution. A typical example is obtained as follows: denote by $\overline{\mathcal{A}}$ another copy of $\mathcal{A}$ and by $\mathcal{A} \ni a \mapsto \overline{a} \in \overline{\mathcal{A}}$ the identity. Then $\mathcal{A} \sqcup \overline{\mathcal{A}}$ has a canonical involution i mapping a to $\overline{a}$ (and hence $\overline{a}$ to a).

One then defines the anti-linear involution $*$ on $\mathfrak{A}(\mathcal{A}, \mathbb{K})$ by

$$(a_1 \cdots a_n)^* = i a_n \cdots i a_1, \quad \mathbb{1}^* = \mathbb{1}.$$

If $\mathfrak{R}$ is invariant under $*$, then $\mathfrak{I}(\mathfrak{R})$ is also a $*$-ideal, and $\mathfrak{A}(\mathcal{A}, \mathbb{K})/\mathfrak{I}(\mathfrak{R})$ is called the *unital* $*$-*algebra with generators* $\mathcal{A}$ *and relations* $R = 0, \quad R \in \mathfrak{R}$. In this case one usually defines the involution $*$ by adding to $\mathfrak{R}$ the elements $a^* - ia$, for $a \in \mathcal{A}$, i.e. by adding the definition of $*$ on the generators to the set of relations.

4.4. States

A *state* on a $*$-algebra $\mathfrak{A}$ is a linear map $\omega : \mathfrak{A} \to \mathbb{C}$ which is *normalized*, i.e. $\omega(\mathbb{1}) = 1$, and *positive*, i.e. $\omega(A^*A) \geq 0$ for $A \in \mathfrak{A}$.

The set of states on $\mathfrak{A}$ is a convex set. Its extreme points are called *pure states*. Note that if $\mathfrak{A} \subset B(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, a state ω on $\mathfrak{A}$ given by $\omega(A) = (\Omega|A\Omega)$ for some unit vector Ω may not be pure.

4.4.1. The GNS (Gelfand-Naimark-Segal) **construction.** If ω is a state on $\mathfrak{A}$, one can perform the so-called GNS *construction*, which we now recall. Let us equip $\mathfrak{A}$ with the scalar product

$$(A|B)_\omega := \omega(A^*B).$$

From the Cauchy-Schwarz inequality one obtains that $\mathfrak{I} = \{A \in \mathfrak{A} : \omega(A^*A) = 0\}$ is a $*$-ideal of $\mathfrak{A}$. We denote by $\mathcal{H}_\omega$ the completion of $\mathfrak{A}/\mathfrak{I}$ for $\|\cdot\|_\omega$ and by $[A] \in \mathcal{H}_\omega$ the image of $A \in \mathfrak{A}$. The fact that $\mathfrak{I}$ is a $*$-ideal implies that for $A \in \mathfrak{A}$ the map

$$\pi_\omega(A) : \mathcal{H}_\omega \ni [B] \longmapsto [AB] \in \mathcal{H}_\omega$$

is well defined and defines a linear operator with $\mathcal{D}_\omega = \{[B] : B \in \mathfrak{A}\}$ as invariant domain. If $\Omega_\omega := [\mathbb{1}]$, then

$$\omega(A) = (\Omega_\omega|\pi_\omega(A)\Omega_\omega)_\omega. \tag{4.2}$$

The triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is called the GNS *triple* associated to ω. It provides a Hilbert space $\mathcal{H}_\omega$, a representation π_ω of $\mathfrak{A}$ by densely defined operators on $\mathcal{H}_\omega$ and a unit vector Ω_ω such that (4.2) holds. Vectors in $\mathcal{H}_\omega$ are physically interpreted as *local excitations* of the ground state Ω_ω.

If $\mathfrak{A}$ is a C^*-algebra, then one can show that $\pi_\omega(A) \in B(\mathcal{H}_\omega)$ with $\|\pi_\omega(A)\| \leq \|A\|$.

4.5. CCR algebras

In this subsection we recall the definition of various $*$-algebras related to the *canonical commutation relations*.

4.5.1. Polynomial CCR **$*$-algebra.**

Definition 4.5.1. *Let $(\mathcal{X}, \sigma)$ be a real pre-symplectic space. The* polynomial CCR $*$-algebra over $(\mathcal{X}, \sigma)$, *denoted by* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$, *is the unital complex $*$-algebra generated by elements $\phi(x)$, $x \in \mathcal{X}$, with relations*

$$\begin{aligned} &\phi(x_1 + \lambda x_2) = \phi(x_1) + \lambda\phi(x_2), \quad \phi^*(x) = \phi(x), \\ &\phi(x_1)\phi(x_2) - \phi(x_2)\phi(x_1) = \mathrm{i}x_1 \cdot \sigma x_2 \mathbb{1}, \end{aligned} \qquad x_1, x_2, x \in \mathcal{X}, \lambda \in \mathbb{R}. \tag{4.3}$$

The elements $\phi(x)$ are called *real* or *selfadjoint fields*.

4.5.2. Weyl CCR **algebra.** One problem with $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ is that its elements cannot be faithfully represented as bounded operators on a Hilbert space. To cure this problem one uses *Weyl operators*, which lead to the Weyl CCR $*$-algebra.

Definition 4.5.2. *The* algebraic Weyl CCR $*$-algebra over $(\mathcal{X}, \sigma)$, *denoted* $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$, *is the $*$-algebra generated by the elements $W(x)$, $x \in \mathcal{X}$, with relations*

$$\begin{aligned} &W(0) = \mathbb{1}, \quad W(x)^* = W(-x), \\ &W(x_1)W(x_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}x_1 \cdot \sigma x_2} W(x_1 + x_2), \end{aligned} \qquad x, x_1, x_2 \in \mathcal{X}. \tag{4.4}$$

The elements $W(x)$ are called *Weyl operators*. An advantage of $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$ is that it can be equipped with a unique C^*-norm see e.g. [**DG**, Definition 8.60]. Its completion for this norm is called the *Weyl* CCR C^**-algebra over* $(\mathcal{X},\sigma)$, and is still denoted by $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$.

We will mostly work with $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$, but it is sometimes important to work with the C^*-algebra $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$, for example in the discussion of pure states, see Section 4.9 below. Of course, the formal relation between the two approaches is

$$W(x)=\mathrm{e}^{\mathrm{i}\phi(x)},\quad x\in\mathcal{X},$$

which does not make sense a priori, but from which mathematically correct statements can be deduced.

4.5.3. Charged CCR **algebra.** Let $(\mathcal{Y},q)$ a pre-Hermitian space. As explained above, we denote the complex structure on $\mathcal{Y}$ by j. The CCR algebra $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}_{\mathbb{R}},\operatorname{Im}q)$ can be generated instead of the selfadjoint fields $\phi(y)$ by the *charged fields*:

$$\psi(y):=\frac{1}{\sqrt{2}}(\phi(y)+\mathrm{i}\phi(\mathrm{j}y)),\quad \psi^*(y):=\frac{1}{\sqrt{2}}(\phi(y)-\mathrm{i}\phi(\mathrm{j}y)),\quad y\in\mathcal{Y}. \tag{4.5}$$

From (4.3) we see that they satisfy the relations

$$\begin{aligned}
&\psi(y_1+\lambda y_2)=\psi(y_1)+\overline{\lambda}\psi(y_2),\\
&\psi^*(y_1+\lambda y_2)=\psi(y_1)+\lambda\psi^*(y_2),\quad y_1,y_2\in\mathcal{Y},\lambda\in\mathbb{C},\\
&[\psi(y_1),\psi(y_2)]=[\psi^*(y_1),\psi^*(y_2)]=0,\\
&[\psi(y_1),\psi^*(y_2)]=\overline{y}_1\cdot qy_2\mathbb{1},\quad y_1,y_2\in\mathcal{Y},\\
&\psi(y)^*=\psi^*(y),\quad y\in\mathcal{Y}.
\end{aligned} \tag{4.6}$$

Note the similarity with the CCR in (3.3) expressed in terms of creation/annihilation operators, the difference being the fact that q is not necessarily positive. The CCR algebra $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}_{\mathbb{R}},\operatorname{Im}q)$ will be denoted by $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},q)$.

4.6. Quasi-free states

In this subsection we discuss states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ or (equivalently) on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$ which are natural for free theories, the so-called *quasi-free states*. We start by discussing general states on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$.

4.6.1. States on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$**.** Let $(\mathcal{X},\sigma)$ be a real pre-symplectic space and ω a state on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$. The function:

$$\mathcal{X}\ni x\longmapsto\omega(W(x))=:G(x) \tag{4.7}$$

is called the *characteristic function* of the state ω, and is an analog of the Fourier transform of a probability measure.

There is also an analog of Bochner's theorem:

Proposition 4.6.1. *A map $G:\mathcal{X}\to\mathbb{C}$ is the characteristic function of a state on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$ iff for any $n\in\mathbb{N}$ and any $x_i\in\mathcal{X}$, the $n\times n$ matrix*

$$\left[G(x_j-x_i)\mathrm{e}^{\frac{\mathrm{i}}{2}x_i\cdot\sigma x_j}\right]_{1\leq i,j\leq n}$$

is positive.

Proof. $\Longrightarrow$ For $x_1, \dots, x_n \in \mathcal{X}$, $\lambda_1, \dots, \lambda_n \in \mathbb{C}$ set $A := \sum_{j=1}^n \lambda_j W(x_j)$. Such A are dense in $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$. One computes A^*A using the CCR and obtains

$$A^*A = \sum_{i,j=1}^n \overline{\lambda}_i \lambda_j W(x_j - x_i) \mathrm{e}^{\frac{\mathrm{i}}{2} x_i \cdot \sigma x_j}, \tag{4.8}$$

from which $\Longrightarrow$ follows.

$\Longleftarrow$ One defines ω using (4.7), and (4.8) shows that ω is positive. □

4.6.2. Quasi-free states on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$.

Definition 4.6.2. *Let $(\mathcal{X}, \sigma)$ be a real pre-symplectic space.*

(1) *A state ω on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ is a* quasi-free state *if there exists $\eta \in L_{\mathrm{s}}(\mathcal{X}, \mathcal{X}')$ such that*

$$\omega\big(W(x)\big) = \mathrm{e}^{-\frac{1}{2} x \cdot \eta x}, \quad x \in \mathcal{X}. \tag{4.9}$$

(2) *The form η is called the* covariance of the quasi-free state ω.

Quasi-free states are generalizations of *Gaussian measures*. In fact, let us assume that $\mathcal{X} = \mathbb{R}^n$ and $\sigma = 0$. $\mathrm{CCR}^{\mathrm{pol}}(\mathbb{R}^n, 0)$ is simply the algebra of complex polynomials on $(\mathbb{R}^n)'$ if we identify $\phi(x)$ with the function $\xi \mapsto x \cdot \xi$. If we consider the Gaussian measure on $(\mathbb{R}^n)'$ with covariance η

$$\mathrm{d}\mu_\eta := (2\pi)^{n/2} (\det \eta)^{-\frac{1}{2}} \mathrm{e}^{-\frac{1}{2} \xi \cdot \eta^{-1} \xi} d\xi,$$

then

$$\int \mathrm{e}^{\mathrm{i} x \cdot \xi} d\mu_\eta(\xi) = \mathrm{e}^{-\frac{1}{2} x \cdot \eta x},$$

which is (4.7). Note also that if $x_i \in \mathbb{R}^n$, then

$$\int \prod_1^{2n+1} x_i \cdot \xi \mathrm{d}\mu_\eta(\xi) = 0,$$

$$\int \prod_1^{2n} x_i \cdot \xi \mathrm{d}\mu_\eta(\xi) = \sum_{\sigma \in \mathrm{Pair}_{2n}} \prod_{j=1}^n x_{\sigma(2j-1)} \cdot \eta x_{\sigma(2j)},$$

which should be compared with Definition 4.6.5 below. We recall that Pair_{2m} denotes the set of *pairings*, i.e. the set of partitions of $\{1, \dots, 2m\}$ into pairs. Any pairing can be written as $\{i_1, j_1\}, \cdots, \{i_m, j_m\}$ for $i_k < j_k$ and $i_k < i_{k+1}$, hence can be uniquely identified with a permutation $\sigma \in S_{2m}$ such that $\sigma(2k-1) = i_k$, $\sigma(2k) = j_k$.

It will be useful later on to collect some properties of the GNS triple associated to a quasi-free state ω on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$, see Subsection 4.4.1. For ease of notation, we omit the subscript ω.

Lemma 4.6.3. *Let us set $W_\pi(x) := \pi(W(x)) \in U(\mathcal{H})$ for $x \in \mathcal{X}$. Then:*

(1) *the one-parameter group $\{W_\pi(tx)\}_{t \in \mathbb{R}}$ is a strongly continuous unitary group on $\mathcal{H}$;*

(2) *let $\phi_\pi(x)$ be its selfadjoint generator. Then $\Omega \in \mathrm{Dom}(\prod_{i=1}^n \phi_\pi(x_i))$ for $n \in \mathbb{N}$, $x_i \in \mathcal{X}$.*

Proof. (1) It suffices to prove the continuity of $t \mapsto W_\pi(tx)u$ for $u \in \mathcal{H}$ at $t = 0$. By density and linearity, we can assume that $u = W_\pi(y)\Omega$, $y \in \mathcal{X}$. Then

$$\|u - W_\pi(tx)u\|^2 = (\Omega | W_\pi(-y)(\mathbb{1} - W_\pi(-tx))(\mathbb{1} - W_\pi(tx)) W_\pi(y)\Omega),$$

and using the CCR (4.4) we have

$$\begin{aligned} W_\pi(-y)(\mathbb{1} - W_\pi(-tx))(\mathbb{1} - W_\pi(tx)) W_\pi(y) \\ = \quad 2\mathbb{1} - W(-tx)\mathrm{e}^{\mathrm{i} t x \cdot \sigma y} - W(tx)\mathrm{e}^{-\mathrm{i} t x \cdot \sigma y}. \end{aligned}$$

Therefore

$$\begin{aligned}\|u - W_\pi(tx)u\|^2 = &\quad \omega(2\mathbb{1} - W(-tx)\mathrm{e}^{\mathrm{i}tx\cdot\sigma y} - W(tx)\mathrm{e}^{-\mathrm{i}tx\cdot\sigma y})\\ = &\quad 2 - \mathrm{e}^{-\frac{1}{2}t^2x\cdot\eta x + \mathrm{i}tx\cdot\sigma y} - \mathrm{e}^{-\frac{1}{2}t^2x\cdot\eta x - \mathrm{i}tx\cdot\sigma y},\end{aligned}$$

which tends to 0 when $t \to 0$.

(2) By [**DG**, Theorem 8.29], it suffices to check that if $\mathcal{X}_{\mathrm{fin}} \subset \mathcal{X}$ is a finite-dimensional subspace, then $\mathcal{X}_{\mathrm{fin}} \ni x \mapsto (\Omega|W_\pi(x)\Omega)$ belongs to the Schwartz class $\mathcal{S}(\mathcal{X}_{\mathrm{fin}})$ of rapidly decaying smooth functions. This is obvious by (4.9). □

Proposition 4.6.4. (1) *One has*

$\mathrm{Dom}\,\phi_\pi(x_1) \cap \mathrm{Dom}\,\phi_\pi(x_2) \subset \mathrm{Dom}\,\phi_\pi(x_1 + x_2)$,

$\phi_\pi(x_1 + x_2) = \phi_\pi(x_1) + \phi_\pi(x_2)$ *on* $\mathrm{Dom}\,\phi_\pi(x_1) \cap \mathrm{Dom}\,\phi_\pi(x_2)$,

$[\phi_\pi(x_1), \phi_\pi(x_2)] = \mathrm{i}x_1\cdot\sigma x_2\mathbb{1}$ *as quadratic forms on* $\mathrm{Dom}\,\phi_\pi(x_1) \cap \mathrm{Dom}\,\phi_\pi(x_2)$.

(2) *One has*

$$(\Omega|\phi_\pi(x_1)\phi_\pi(x_2)\Omega) = x_1\cdot\eta x_2 + \frac{\mathrm{i}}{2}x_1\cdot\sigma x_2, \quad x_1, x_2 \in \mathcal{X}. \tag{4.10}$$

(3) *One has*

$$(\Omega|\phi_\pi(x_1)\cdots\phi_\pi(x_{2m-1})\Omega) = 0, \tag{4.11}$$

$$(\Omega|\phi_\pi(x_1)\cdots\phi_\pi(x_{2m})\Omega) = \sum_{\sigma\in\mathrm{Pair}_{2m}}\prod_{j=1}^{m}(\Omega|\phi_\pi(x_{\sigma(2j-1)})\phi_\pi(x_{\sigma(2j)})\Omega). \tag{4.12}$$

Proof. (1) follows from [**DG**, Theorem 8.25].

(2) We have $(\Omega|W_\pi(tx)\Omega) = \mathrm{e}^{-\frac{1}{2}t^2x\eta x}$, which when differentiated twice with respect to t at $t = 0$ gives $(\Omega|\phi_\pi^2(x)\Omega) = x\cdot\eta x$. We then apply (1), i.e. linearity and the CCR to obtain (4.10).

(3) $\mathrm{i}^n(\Omega|\phi_\pi(x_1)\cdots\phi_\pi(x_n)\Omega)$ is the coefficient of $t_1\cdots t_n$ in the power series expansion of $\omega(W(t_1x_1)\cdots W(t_nx_n))$. One then uses the CCR and (4.9) to compute this function. Details can be found e.g. in [**DG**, Proposition 17.8]. □

4.6.3. Quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$. From Proposition 4.6.4 one sees that a quasi-free state ω on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma)$ induces a state $\tilde{\omega}$ on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ by setting

$$\tilde{\omega}(\prod_{i=1}^{n}\phi(x_i)) := (\Omega|\prod_{i=1}^{n}\phi_\pi(x_i)\Omega).$$

Indeed, $\tilde{\omega}$ is well defined on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ since it vanishes on elements of the ideal $\mathfrak{I}(\mathfrak{R})$ for $\mathfrak{R}$ introduced in (4.3), by Proposition 4.6.4 (1).

This leads to the following definition of quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$.

Definition 4.6.5. (1) *A state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ is* quasi-free *if for any $m \in \mathbb{N}$ and $x_i \in \mathcal{X}$ one has*

$$\omega\big(\phi(x_1)\cdots\phi(x_{2m-1})\big) = 0, \tag{4.13}$$

$$\omega\big(\phi(x_1)\cdots\phi(x_{2m})\big) = \sum_{\sigma\in\mathrm{Pair}_{2m}}\prod_{j=1}^{m}\omega\big(\phi(x_{\sigma(2j-1)})\phi(x_{\sigma(2j)})\big). \tag{4.14}$$

(2) *The symmetric form $\eta \in L_{\mathrm{s}}(\mathcal{X},\mathcal{X}')$ defined by*

$$\omega(\phi(x_1)\phi(x_2)) =: x_1\cdot\eta x_2 + \frac{\mathrm{i}}{2}x_1\cdot\sigma x_2 \tag{4.15}$$

is called the covariance *of the state ω.*

4.7. Covariances of quasi-free states

PROPOSITION 4.7.1. *Let $\eta \in L_{\rm s}(\mathcal{X}, \mathcal{X}')$. Then the following are equivalent:*

(1) *there exists a quasi-free state ω on $\mathrm{CCR}^{\mathrm{Weyl/pol}}(\mathcal{X}, \sigma)$ with covariance η.*
(2) *$\eta_{\mathbb{C}} + \frac{\mathrm{i}}{2}\sigma_{\mathbb{C}} \geq 0$ on $\mathbb{C}\mathcal{X}$, where $\eta_{\mathbb{C}}, \sigma_{\mathbb{C}} \in L(\mathbb{C}\mathcal{X}, (\mathbb{C}\mathcal{X})^*)$ are the sesquilinear extensions of η, σ.*
(3) *$\eta \geq 0$ and $|x_1 \cdot \sigma x_2| \leq 2(x_1 \cdot \eta x_1)^{\frac{1}{2}}(x_2 \cdot \eta x_2)^{\frac{1}{2}}$, $x_1, x_2 \in \mathcal{X}$.*

Proof. (1) $\Longrightarrow$ (2) If η is the covariance of a state ω on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ one introduces complex fields $\phi_\pi(w) = \phi_\pi(x_1) + \mathrm{i}\phi_\pi(x_2)$, $w = x_1 + \mathrm{i}x_2 \in \mathbb{C}\mathcal{X}$ with domain $\mathrm{Dom}\,\phi_\pi(x_1) \cap \mathrm{Dom}\,\phi_\pi(x_2)$. By Proposition 4.6.4, $(\phi_\pi(w)\Omega|\phi_\pi(w)\Omega)$ is well defined, positive, and equals $\overline{w} \cdot (\eta_{\mathbb{C}} + \frac{\mathrm{i}}{2}\sigma_{\mathbb{C}})w$. The same argument, with $\phi_\pi(\cdot)$ replaced by $\phi(\cdot)$, gives the proof for $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$.

(2) $\Longrightarrow$ (1) Let us fix $x_1, \ldots, x_n \in \mathcal{X}$ and set $b_{ij} = x_i \cdot \eta x_j + \frac{\mathrm{i}}{2} x_i \cdot \sigma x_j$. Then, for $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$,

$$\sum_{i,j=1}^{n} \overline{\lambda_i} b_{ij} \lambda_j = \overline{w} \cdot \eta_{\mathbb{C}} w + \tfrac{\mathrm{i}}{2} \overline{w} \cdot \omega_{\mathbb{C}} w, \quad w = \sum_{i=1}^{n} \lambda_i x_i \in \mathbb{C}\mathcal{X}.$$

By (2), the matrix $\left[b_{ij}\right]$ is positive. The pointwise product of two positive matrices is positive, see e.g. [**DG**, Proposition 17.6], which implies that $\left[\mathrm{e}^{b_{ij}}\right]$ is positive, and hence $\left[\mathrm{e}^{-\frac{1}{2}x_i \cdot \eta x_i} \mathrm{e}^{b_{ij}} \mathrm{e}^{-\frac{1}{2}x_j \cdot \eta x_j}\right]$ is positive. This matrix equals $\left[G(x_j - x_i)\mathrm{e}^{\frac{\mathrm{i}}{2}x_i \cdot \sigma x_j}\right]$ with $G(x) = \mathrm{e}^{-\frac{1}{2}x \cdot \eta x}$. By Proposition 4.6.1, η is the covariance of a quasi-free state on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$. By the discussion following Subsection 4.6.3, it is also the covariance of a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$.

The proof of (2) $\Longleftrightarrow$ (3) is an exercise in linear algebra. □

We will identify in the sequel the two states on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ and $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ having the same covariance η.

4.7.1. Quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$. Let now $(\mathcal{Y}, q)$ a pre-Hermitian space. Recall that if $\mathcal{X} = \mathcal{Y}_{\mathbb{R}}$ and $\sigma = \mathrm{Im}\, q$, then $(\mathcal{X}, \sigma)$ is a real pre-symplectic space, and by definition $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q) = \mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$.

The complex structure j of $\mathcal{Y}$ belongs to $Sp(\mathcal{X}, \sigma)$ and also to $sp(\mathcal{X}, \sigma)$ since $\mathrm{j}^2 = -\mathbb{1}$. It follows that $\{\mathrm{e}^{\mathrm{j}\theta}\}_{\theta \in \mathbb{S}^1}$ is a one-parameter group of symplectic transformations.

Therefore, one can define a group $\{\alpha_\theta\}_{\theta \in \mathbb{S}^1}$ of automorphisms of $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ by

$$\alpha_\theta \phi(x) := \phi(\mathrm{e}^{\mathrm{j}\theta} x). \tag{4.16}$$

The gauge transformations α_θ are *global* gauge transformations, which should not be confused with the local gauge transformations arising for example in electromagnetism.

DEFINITION 4.7.2. *A quasi-free state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ is called* gauge invariant *if*

$$\omega(\alpha_\theta(A)) = \omega(A), \quad A \in \mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma),\ \theta \in \mathbb{S}^1.$$

The following lemma follows immediately from Definition 4.7.2.

LEMMA 4.7.3. *A quasi-free state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ with covariance η is gauge invariant iff $\mathrm{j} \in O(\mathcal{X}, \eta)$ iff $\mathrm{j} \in o(\mathcal{X}, \eta)$. One can then define $\hat{\eta} \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$ by*

$$\overline{y}_1 \cdot \hat{\eta} y_2 := y_1 \cdot \eta y_2 - \mathrm{i} y_1 \cdot \eta \mathrm{j} y_2, \quad y_1, y_2 \in \mathcal{Y}. \tag{4.17}$$

It is then natural to consider the action of ω on products of the charged fields $\psi(y), \psi^*(y)$ introduced in (4.5). Note that by the CCR (4.6), ω is completely determined by its action on elements

$$A = \prod_{i=1}^{n} \psi^*(y_i) \prod_{j=1}^{m} \psi(y'_j). \tag{4.18}$$

PROPOSITION 4.7.4. *A quasi-free state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$ is gauge invariant iff*

$$\omega(\prod_{i=1}^{n} \psi^*(y_i) \prod_{j=1}^{m} \psi(y'_j)) = 0, \text{ if } n \neq m, \tag{4.19}$$

$$\omega(\prod_{i=1}^{n} \psi^*(y_i) \prod_{j=1}^{n} \psi(y'_j)) = \sum_{\sigma \in S_n} \prod_{i=1}^{n} \omega(\psi^*(y_i)\psi(y'_{\sigma(i)})). \tag{4.20}$$

Proof. Using that $\alpha_\theta(\psi^*(y)) = \mathrm{e}^{\mathrm{j}\theta}\psi^*(y)$, we obtain that if A is as in (4.18) $\alpha_\theta(A) = \mathrm{e}^{\mathrm{j}(n-m)\theta}A$, which implies (4.19). The proof of (4.20) is a routine computation, using (4.5) and Definition 4.6.5. □

DEFINITION 4.7.5. *The sesquilinear forms $\lambda^{\pm} \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$ defined by*

$$\begin{aligned} \omega(\psi(y_1)\psi^*(y_2)) &=: \quad \overline{y}_1 \cdot \lambda^+ y_2, \\ \omega(\psi^*(y_2)\psi(y_1)) &=: \quad \overline{y}_1 \cdot \lambda^- y_2, \quad y_1, y_2 \in \mathcal{Y}, \end{aligned} \tag{4.21}$$

are called the complex covariances *of the quasi-free state ω.*

Note that since $[\psi(y_1), \psi^*(y_2)] = \overline{y}_1 \cdot q y_2 \mathbb{1}$, we have $\lambda^+ - \lambda^- = q$. Therefore ω is completely determined by either λ^+ or λ^-. Nevertheless, it is more convenient to consider the pair $\lambda^{\pm}$ when discussing properties of ω. λ^- is usually called the *charge density* associated to ω.

Introducing the selfadjoint fields $\phi(y)$, we obtain that

$$\omega(\phi(y_1)\phi(y_2)) = \mathrm{Re}(\overline{y}_1 \cdot (\lambda^+ - \frac{1}{2}q)y_2) + \frac{\mathrm{i}}{2}\mathrm{Im}(\overline{y}_1 \cdot q y_2). \tag{4.22}$$

It follows that the real and complex covariances of a gauge invariant quasi-free state are connected by the relations

$$\eta = \mathrm{Re}(\lambda^{\pm} \mp \frac{1}{2}q), \quad \lambda^{\pm} = \hat{\eta} \pm \frac{1}{2}q, \tag{4.23}$$

where $\hat{\eta}$ is defined in (4.17).

In this situation we will call η the *real covariance* of the state ω, to distinguish it from the complex covariances $\lambda^{\pm}$.

It is easy to characterize the complex covariances of a gauge invariant quasi-free state.

PROPOSITION 4.7.6. *Let $\lambda^{\pm} \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$. Then the following are equivalent:*
(1) *$\lambda^{\pm}$ are the covariances of a gauge invariant quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$;*
(2) *$\lambda^{\pm} \geq 0$ and $\lambda^+ - \lambda^- = q$.*

Proof. The implication (1) $\Longrightarrow$ (2) is immediate using the CCR and the fact that $\psi(y)\psi^*(y)$ and $\psi^*(y)\psi(y)$ are positive. Let us now prove that (2) $\Longrightarrow$ (1). We recall that $\mathcal{X} = \mathcal{Y}_{\mathbb{R}}$. Let η be the real covariance of a gauge invariant quasi-free state. For $x \in \mathcal{X}$ let $z = \frac{1}{\sqrt{2}}(x - \mathrm{ij}x), \overline{z} = \frac{1}{\sqrt{2}}(x + \mathrm{ij}x)$. We know that $\mathrm{j} \in O(\mathcal{X}, \eta) \cap o(\mathcal{X}, \eta)$, which after a standard computation yields

$$\begin{aligned} (\overline{z}|\eta_{\mathbb{C}} z) &= x \cdot \eta x - \mathrm{i}x \cdot \eta \mathrm{j} x = \overline{x} \cdot \hat{\eta} x, \\ (z|\eta_{\mathbb{C}} \overline{z}) &= x \cdot \eta x - \mathrm{i}x \cdot \eta \mathrm{j} x = \overline{x} \cdot \hat{\eta} x. \end{aligned} \tag{4.24}$$

Similarly, using that $\mathrm{j} \in Sp(\mathcal{X},\sigma) \cap sp(\mathcal{X},\sigma)$ we obtain

$$\begin{aligned}(\overline{z}|\sigma_{\mathbb{C}} z) &= x\cdot\sigma x - \mathrm{i}x\cdot\sigma \mathrm{j} x = -\mathrm{i}\overline{x}\cdot q x,\\ (z|\sigma_{\mathbb{C}}\overline{z}) &= x\cdot\sigma x + \mathrm{i}x\cdot\sigma \mathrm{j} x = \mathrm{i}\overline{x}\cdot q x.\end{aligned} \tag{4.25}$$

By Proposition 4.7.1 (2) we have $\eta_{\mathbb{C}} + \frac{\mathrm{i}}{2}\sigma_{\mathbb{C}} \geq 0$, which implies that $\hat{\eta} \pm \frac{1}{2} q = \lambda^{\pm} \geq 0$. The fact that $\lambda^+ - \lambda^- = q$ follows from (4.23). □

4.7.2. Complexification of a quasi-free state. Let $(\mathcal{X},\sigma)$ be a real pre-symplectic space. We equip $\mathbb{C}\mathcal{X}$ with $q = \mathrm{i}\sigma_{\mathbb{C}}$, obtaining a pre-Hermitian space. The canonical complex conjugation on $\mathbb{C}\mathcal{X}$ is a charge reversal on $(\mathbb{C}\mathcal{X}, q)$.

Clearly $((\mathbb{C}\mathcal{X})_{\mathbb{R}}, \operatorname{Im} q)$ is isomorphic to $(\mathcal{X}\oplus\mathcal{X}, \sigma\oplus\sigma)$ as real pre-symplectic spaces. If ω is a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ with covariance η, then we can consider the quasi-free state $\tilde{\omega}$ on $\mathrm{CCR}^{\mathrm{pol}}(\mathbb{C}\mathcal{X})_{\mathbb{R}}, \operatorname{Im} q)$ with covariance $\operatorname{Re}\eta_{\mathbb{C}}$.

It is easy to see that $\tilde{\omega}$ is gauge invariant with covariances $\lambda^{\pm}$ equal to

$$\lambda^{\pm} = \eta_{\mathbb{C}} \pm \frac{1}{2} q. \tag{4.26}$$

Moreover, $\tilde{\omega}$ is invariant under charge reversal.

Therefore, by complexifying a quasi-free state ω on a real pre-symplectic space $(\mathcal{X},\sigma)$, we obtain a gauge invariant quasi-free state $\tilde{\omega}$ on $\mathcal{A}(\mathbb{C}\mathcal{X},\sigma_{\mathbb{C}})$. It follows that, possibly after complexifying the real pre-symplectic space $(\mathcal{X},\sigma)$, one can always restrict the discussion to gauge invariant quasi-free states.

Remark 4.7.7. *Let $(\mathcal{Y}, q)$ pre-Hermitian and ω a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$. Assume that ω is* not gauge invariant. *This means that the complex structure* j *of $\mathcal{Y}$ is irrelevant for the analysis of ω and hence can be forgotten.*

Therefore, we consider ω simply as a quasi-free state on the real pre-symplectic space $(\mathcal{X},\sigma) = (\mathcal{Y}_{\mathbb{R}}, \operatorname{Im} q)$. If we want to recover a gauge invariant quasi-free state, we consider the state $\tilde{\omega}$ on $\mathrm{CCR}^{\mathrm{pol}}(\mathbb{C}\mathcal{X}, \mathrm{i}\sigma_{\mathbb{C}})$.

4.8. The GNS representation of quasi-free states

Let us now discuss the GNS representation of a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$. We will assume for simplicity that its real covariance η is non degenerate, i.e. $\operatorname{Ker}\eta = \{0\}$. From Proposition 4.7.1 (3) we see that $\operatorname{Ker}\eta \subset \operatorname{Ker}\sigma$, hence in particular $\operatorname{Ker}\eta = \{0\}$ if σ is symplectic.

Let $\mathcal{X}^{\mathrm{cpl}}$ the completion of $\mathcal{X}$ for $(x\cdot\eta x)^{\frac{1}{2}}$, which is a real Hilbert space. The extension σ^{cpl} is bounded on $\mathcal{X}^{\mathrm{cpl}}$, but may be degenerate on $\mathcal{X}^{\mathrm{cpl}}$. Moreover, ω induces a unique quasi-free state ω^{cpl} on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}^{\mathrm{cpl}}, \sigma^{\mathrm{cpl}})$.

To simplify notation, we forget the superscripts cpl in this subsection and assume that $\mathcal{X}$ is complete for $(x\cdot\eta x)^{\frac{1}{2}}$.

The GNS representation was first constructed by Manuceau and Verbeure [**MV**] in the case where σ is non-degenerate. Its extension to the general case was given by Kay and Wald [**KW**, Appendix A], where it was called a *one-particle Hilbert space structure*. Another equivalent representation if σ is non-degenerate is called the *Araki-Woods* representation, see [**AW**].

An important fact in this context is the following result, due to Leyland, Roberts and Testard [**LRT**, Theorem 1.3.2], about dense subspaces of a Fock space $\Gamma_{\mathrm{s}}(\mathfrak{h})$. Another proof can be deduced from the results in [**DG**, Section 17.3].

Theorem 4.8.1. *Let $\mathfrak{h}$ a complex Hilbert space and $\mathcal{X} \subset \mathfrak{h}$ a real vector subspace. Then the space $\mathrm{Vect}\{W_{\mathrm{F}}(x)\Omega_{\mathrm{vac}} : x \in \mathcal{X}\}$ is dense in $\Gamma_{\mathrm{s}}(\mathfrak{h})$ iff $\mathbb{C}\mathcal{X}$ is dense in $\mathfrak{h}$.*

Note that if we denote by $\mathcal{X}^{\perp}$, resp. $\mathcal{X}^{\mathrm{perp}}$ the space orthogonal to $\mathcal{X}$ with respect to the scalar product $(\cdot|\cdot)_{\mathfrak{h}}$, resp. $\mathrm{Re}(\cdot|\cdot)_{\mathfrak{h}}$, we have $(\mathrm{i}\mathcal{X})^{\mathrm{perp}} = \mathrm{i}\mathcal{X}^{\mathrm{perp}}$, $\mathcal{X}^{\perp} = \mathcal{X}^{\mathrm{perp}} \cap \mathrm{i}\mathcal{X}^{\mathrm{perp}}$ and $\mathrm{i}\mathcal{X}^{\mathrm{perp}}$ is also the space orthogonal to $\mathcal{X}$ with respect to the symplectic form $\sigma = \mathrm{Im}\,(\cdot|\cdot)_{\mathfrak{h}}$. Therefore, an equivalent condition in Theorem 4.8.1 is that $\mathcal{X}^{\mathrm{perp}} \cap \mathrm{i}\mathcal{X}^{\mathrm{perp}} = \{0\}$.

4.8.1. Kähler structures.

PROPOSITION 4.8.2. *Let η be the real covariance of a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ such that η is non-degenerate and $\mathcal{X}$ is complete for $(x\cdot\eta x)^{\frac{1}{2}}$. Then if $\dim \mathrm{Ker}\,\sigma$ is even or infinite, there exists an anti-involution j on $\mathcal{X}$ such that (η,j) is Kähler.*

Proof. By Proposition 4.7.1 (3), there exists a bounded anti-symmetric operator $c \in L_{\mathrm{a}}(\mathcal{X})$ with $\|c\| \leq 1$ such that

$$\sigma = 2\eta c. \tag{4.27}$$

We have of course $\mathrm{Ker}\, c = \mathrm{Ker}\,\sigma$ and we set $\mathcal{X}_{\mathrm{sing}} := \mathrm{Ker}\, c$, $\mathcal{X}_{\mathrm{reg}} := \mathcal{X}_{\mathrm{sing}}^{\perp}$. Since c is anti-symmetric, it preserves $\mathcal{X}_{\mathrm{reg}}$ and $\mathcal{X}_{\mathrm{sing}}$. If c_{reg} is the restriction of c to $\mathcal{X}_{\mathrm{reg}}$ then one can perform its polar decomposition $c_{\mathrm{reg}} = -\mathrm{j}_{\mathrm{reg}}|c|_{\mathrm{reg}}$, and using the anti-symmetry of c_{reg} one obtain that $\mathrm{j}_{\mathrm{reg}}^2 = -\mathbb{1}$, $\mathrm{j}_{\mathrm{reg}} \in O(\mathcal{X}_{\mathrm{reg}},\eta)$ and $[|c_{\mathrm{reg}}|,\mathrm{j}_{\mathrm{reg}}] = 0$, see e.g. [**DG**, Proposition 2.84].

Since $\dim \mathcal{X}_{\mathrm{sing}}$ is even or infinite, we can choose an arbitrary anti-involution $\mathrm{j}_{\mathrm{sing}} \in O(\mathcal{X}_{\mathrm{sing}},\eta)$. Then $\mathrm{j} = \mathrm{j}_{\mathrm{reg}} \oplus \mathrm{j}_{\mathrm{sing}}$ has the required properties. □

4.8.2. The GNS representation. Let us equip $\mathcal{X}$ with a complex structure j as in Proposition 4.8.2, and with the scalar product

$$(x_1|x_2)_{\mathrm{KW}} := x_1\cdot\eta x_2 - \mathrm{i}x_1\cdot\eta\mathrm{j}x_2. \tag{4.28}$$

The completion of $\mathcal{X}$ for this scalar product is denoted by $\mathcal{X}_{\mathrm{KW}}$ in the sequel. We set

$$\mathfrak{h}_{\mathrm{KW}} := \mathcal{X}_{\mathrm{KW}} \oplus \mathbb{1}_{\mathbb{R}\setminus\{1\}}(|\overline{c}|)\overline{\mathcal{X}_{\mathrm{KW}}},$$

where c is as in (4.27) and

$$\phi_{\mathrm{KW}}(x) = \phi_{\mathrm{F}}((1+|c|)^{\frac{1}{2}}x \oplus (1-\overline{|c|})^{\frac{1}{2}}\overline{x}),\ x \in \mathcal{X}. \tag{4.29}$$

acting on $\Gamma_{\mathrm{s}}(\mathfrak{h}_{\mathrm{KW}})$.

PROPOSITION 4.8.3. *The triple $(\mathcal{H}_{\mathrm{KW}},\pi_{\mathrm{KW}},\Omega_{\mathrm{KW}})$, defined by*

$$\mathcal{H}_{\mathrm{KW}} = \Gamma_{\mathrm{s}}(\mathfrak{h}_{\mathrm{KW}}),\quad \pi_{\mathrm{KW}}\phi(x) = \phi_{\mathrm{KW}}(x),\quad x \in \mathcal{X},\quad \Omega_{\mathrm{KW}} = \Omega_{\mathrm{vac}},$$

is the GNS *triple of the quasi-free state ω.*

Proof. Using (4.28) we check by standard computations that

$$[\phi_{\mathrm{KW}}(x_1),\phi_{\mathrm{KW}}(x_2)] = \mathrm{i}\mathrm{Im}\,(x_1|x_2)_{\mathfrak{h}_{\mathrm{KW}}} = \mathrm{i}x_1\cdot\sigma x_2,$$
$$(\Omega_{\mathrm{vac}}|\phi_{\mathrm{KW}}(x_1)\phi_{\mathrm{KW}}(x_2)\Omega_{\mathrm{vac}}) = x_1\cdot\eta x_2 + \tfrac{\mathrm{i}}{2}x_1\cdot\sigma x_2.$$

Using the CCR on $\Gamma_{\mathrm{s}}(\mathfrak{h}_{\mathrm{KW}})$, we then check that $\omega(A) = (\Omega_{\mathrm{vac}}|\pi(A)\Omega_{\mathrm{vac}})$ for all $A \in \mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$.

It remains to prove that $\pi_{\mathrm{KW}}(\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X},\sigma))\Omega_{\mathrm{KW}}$ is dense in $\mathcal{H}_{\mathrm{KW}}$, i.e. by Theorem 4.8.1, that $\mathbb{C}R\mathcal{X}$ is dense in $\mathfrak{h}_{\mathrm{KW}}$ for $Rx = (1+|c|)^{\frac{1}{2}}x \oplus (1-\overline{|c|})^{\frac{1}{2}}\overline{x}$. This follows easily from the fact that the complex structure on $\mathfrak{h}_{\mathrm{KW}}$ is $\mathrm{j} \oplus -\mathrm{j}$. □

If σ is non-degenerate, another equivalent version of the GNS representation is given by the *Araki-Woods* representation: one equips $\mathcal{X}$ with the complex structure $\mathrm{j} = -c|c|^{-1}$ given in Proposition 4.8.2, and with the scalar product

$$(x_1|x_2)_{\mathrm{AW}} := x_1\cdot\sigma\mathrm{j}x_2 + \mathrm{i}x_1\cdot\sigma x_2. \tag{4.30}$$

The completion of $\mathcal{X}$ for this scalar product is denoted by $\mathcal{X}_{\rm AW}$ and equals to $|c|^{-\frac{1}{2}}\mathcal{X}_{\rm KW}$, w ith the notation introduced in Subsection1.3.1. One sets then

$$\varrho = \frac{1-|c|}{|c|}$$

as a (possibly unbounded) operator on $\mathcal{X}_{\rm AW}$. From (4.27), (4.30) we obtain that $(x|\varrho x)_{\rm AW} = x\cdot\eta x$, hence $\mathcal{X} \subset \mathrm{Dom}\,\varrho^{\frac{1}{2}}$. The *Araki-Woods representation* is then obtained by setting

$$\mathfrak{h}_{\rm AW} = \mathcal{X}_{\rm AW} \oplus \mathbb{1}_{\mathbb{R}\setminus\{1\}}(|c|)\overline{\mathcal{X}_{\rm AW}},$$

and defining the *left Araki-Woods representation*

$$\phi_{\rm AW,l}(x) := \phi_{\rm F}((1+\varrho)^{\frac{1}{2}}x \oplus \overline{\varrho}^{\frac{1}{2}}\overline{x}), \quad x \in \mathcal{X}. \tag{4.31}$$

Setting

$$\mathcal{H}_{\rm AW} = \Gamma_{\rm s}(\mathfrak{h}_{\rm AW}), \quad \pi_{\rm AW,l}\phi(x) = \phi_{\rm AW,l}(x), \quad x \in \mathcal{X}, \quad \Omega_{\rm AW} = \Omega_{\rm vac},$$

one can show by the same arguments that $(\mathcal{H}_{\rm AW}, \pi_{\rm AW,l}, \Omega_{\rm AW})$ is an equivalent GNS representation for ω.

4.8.3. Doubling procedure. Let us assume that $\mathbb{1}_{\{1\}}(|c|) = 0$, i.e. $\mathfrak{h}_{\rm AW} = \mathcal{X}_{\rm AW} \oplus \overline{\mathcal{X}}_{\rm AW}$. One defines the *right Araki-Woods representation*

$$\phi_{\rm AW,r}(x) := \phi_{\rm F}(\varrho^{\frac{1}{2}}x \oplus (1+\overline{\varrho})^{\frac{1}{2}}\overline{x}), \quad x \in \mathcal{X},$$

which satisfies

$$[\phi_{\rm AW,r}(x_1), \phi_{\rm AW,r}(x_2)] = -{\rm i}x_1\cdot\sigma x_2, \quad [\phi_{\rm AW,l}(x_1), \phi_{\rm AW,r}(x_2)] = 0, \quad x_1, x_2 \in \mathcal{X}.$$

One can now combine the left and right Araki-Woods representations by doubling the phase space. This doubling procedure is due to Kay **[Ky2]**. One sets

$$(\mathcal{X}_{\rm d}, \sigma_{\rm d}) := (\mathcal{X}, \sigma) \oplus (\mathcal{X}, -\sigma),$$
$$\phi_{\rm d}(x_{\rm d}) := \phi_{\rm AW,l}(x) + \phi_{\rm AW,r}(x'), \quad x_{\rm d} = (x, x') \in \mathcal{X}_{\rm d},$$

and the vacuum vector $\Omega_{\rm vac}$ induces a quasi-free state $\omega_{\rm d}$ on $\mathrm{CCR}^{\rm pol}(\mathcal{X}_{\rm d}, \sigma_{\rm d})$ by

$$\omega_{\rm d}(\phi(x_{1,d})\phi(x_{2,d})) = (\Omega_{\rm vac}|\phi_{\rm d}(x_{1,d})\phi_{\rm d}(x_{2,d})\Omega_{\rm vac})_{\mathcal{H}_{\rm AW}}.$$

This state is a *pure state*, see Section 4.9. If we embed $\mathrm{CCR}^{\rm pol}(\mathcal{X}, \sigma)$ into $\mathrm{CCR}^{\rm pol}(\mathcal{X}_{\rm d}, \sigma_{\rm d})$ by the map $\mathcal{X} \ni x \mapsto (x, 0) \in \mathcal{X}_{\rm d}$, then the restriction of $\omega_{\rm d}$ to $\mathrm{CCR}^{\rm pol}(\mathcal{X}, \sigma)$ equals ω.

4.8.4. Charged versions. Let us now describe the complex versions of the above constructions.

Let $\lambda^{\pm}$ be the complex covariances of a quasi-free state on $\mathrm{CCR}^{\rm pol}(\mathcal{Y}, q)$. Assume that $\lambda^+ + \lambda^-$ is non-degenerate, which is the case if q is non-degenerate, and that $\mathcal{Y}$ is complete for the scalar product $\lambda^+ + \lambda^-$. Then there exists $d \in L_{\rm h}(\mathcal{Y})$ with $\|d\| \leq 1$ such that

$$q = (\lambda^+ + \lambda^-)d. \tag{4.32}$$

Setting $\mathcal{X} = \mathcal{Y}_{\mathbb{R}}$, we have $\eta = \frac{1}{2}\mathrm{Re}(\lambda^+ + \lambda^-)$ and $\sigma = \mathrm{Im}\,q$ which implies that the operator c in Proposition 4.8.2 equals $-{\rm i}d$ and hence that ${\rm j}_{\rm reg} = {\rm isgn}(d)$. Since $\mathrm{Ker}\,\sigma = \mathrm{Ker}\,q$, its (real) dimension is even or infinite.

Assuming for simplicity that $\mathrm{Ker}\,d = \{0\}$ we can rewrite $(\cdot|\cdot)_{\rm KW}$ as

$$2(y_1|y_2)_{\rm KW} = \overline{y}_1\cdot(\lambda^+ + \lambda^-)\mathbb{1}_{\mathbb{R}^+}(d)y_2 + \overline{y}_2\cdot(\lambda^+ + \lambda^-)\mathbb{1}_{\mathbb{R}^-}(d)y_1. \tag{4.33}$$

Similarly, we can rewrite $(\cdot|\cdot)_{\rm AW}$ as

$$(y_1|y_2)_{\rm AW} = \overline{y}_1\cdot q\mathbb{1}_{\mathbb{R}^+}(d)y_2 - \overline{y}_2\cdot q\mathbb{1}_{\mathbb{R}^-}(d)y_1.$$

Finally, let us discuss the doubling procedure in the charged case. We start from a Hermitian space $(\mathcal{Y}, q)$ and consider

$$(\mathcal{Y}_{\mathrm{d}}, q_{\mathrm{d}}) := (\mathcal{Y} \oplus \mathcal{Y}, q \oplus -q).$$

Let us denote by $\lambda_{\mathrm{d}}^{\pm}$ the complex covariances of the doubled state ω_{d}. One can show, see e.g. [**G2**, Subsection 5.4] that

$$\lambda_{\mathrm{d}}^{\pm} = \pm q_{\mathrm{d}} \circ c_{\mathrm{d}}^{\pm},$$

where

$$\begin{aligned} c_{\mathrm{d}}^{+} &= \begin{pmatrix} (\varrho+1)\mathbb{1}_{\mathbb{R}^+}(d) - \varrho\mathbb{1}_{\mathbb{R}^-}(d) & -\varrho^{\frac{1}{2}}(\varrho+1)^{\frac{1}{2}}\mathrm{sgn}(d) \\ \varrho^{\frac{1}{2}}(\varrho+1)^{\frac{1}{2}}\mathrm{sgn}(d) & -\varrho\mathbb{1}_{\mathbb{R}^+}(d) + (\varrho+1)\mathbb{1}_{\mathbb{R}^-}(d) \end{pmatrix}, \\ c_{\mathrm{d}}^{-} &= \begin{pmatrix} -\varrho\mathbb{1}_{\mathbb{R}^+}(d) + (\varrho+1)\mathbb{1}_{\mathbb{R}^-}(d) & \varrho^{\frac{1}{2}}(\varrho+1)^{\frac{1}{2}}\mathrm{sgn}(d) \\ -\varrho^{\frac{1}{2}}(\varrho+1)^{\frac{1}{2}}\mathrm{sgn}(d) & (\varrho+1)\mathbb{1}_{\mathbb{R}^+}(d) - \varrho\mathbb{1}_{\mathbb{R}^-}(d) \end{pmatrix}, \end{aligned} \tag{4.34}$$

where d is defined above and $\varrho = \frac{1-|d|}{|d|}$. One can check that $c_{\mathrm{d}}^{\pm}$ are a pair of complementary projections, which is related to the fact that ω_{d} is a pure state.

4.9. Pure quasi-free states

Let us now discuss *pure* quasi-free states, which are often called *vacuum states* in physics. We will always assume that $(\mathcal{X}, \sigma)$ is pre-symplectic, and the covariance η is non-degenerate.

A basic result, see e.g. [**BR**, Theorem 2.3.19], says that a state ω on a C^*-algebra $\mathfrak{A}$ is pure iff its GNS representation $(\mathcal{H}_\omega, \pi_\omega)$ is irreducible, i.e. iff $\mathcal{H}_\omega$ does not contain non-trivial closed subspaces, invariant under $\pi_\omega(\mathfrak{A})$.

To be able to apply this result, we will say that a quasi-free state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ is pure if it is pure as a state on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$.

4.9.1. Pure quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$. We use the notation $\mathcal{X}^{\mathrm{cpl}}, \sigma^{\mathrm{cpl}}, \omega^{\mathrm{cpl}}$ introduced in Section 4.8.

Proposition 4.9.1. *A quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ with covariance η is pure iff $(2\eta^{\mathrm{cpl}}, \sigma^{\mathrm{cpl}})$ is Kähler, i.e. there exists an anti-involution $\mathrm{j}^{\mathrm{cpl}} \in Sp(\mathcal{X}^{\mathrm{cpl}}, \sigma^{\mathrm{cpl}})$ such that $\sigma^{\mathrm{cpl}}\mathrm{j}^{\mathrm{cpl}} = 2\eta^{\mathrm{cpl}}$.*

Note that this implies that σ^{cpl} is non-degenerate on $\mathcal{X}^{\mathrm{cpl}}$. Equivalent characterizations of pure quasi-free states are given in [**MV**, Proposition 12] or [**KW**, Lemma A.2].

Proof. Let us set $\mathfrak{A}^{(\mathrm{cpl})} = \mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}^{(\mathrm{cpl})}, \sigma^{(\mathrm{cpl})})$ and let $(\mathcal{H}^{(\mathrm{cpl})}, \pi^{(\mathrm{cpl})}, \Omega^{(\mathrm{cpl})})$ be the GNS triple for $\omega^{(\mathrm{cpl})}$. Using that $\mathcal{X}$ is dense in $\mathcal{X}^{\mathrm{cpl}}$ for η, we first obtain that $\mathcal{H} = \mathcal{H}^{\mathrm{cpl}}$, $\Omega = \Omega^{\mathrm{cpl}}$ and $\pi^{\mathrm{cpl}}|_{\mathfrak{A}} = \pi$.

We then claim that $\pi(\mathfrak{A})$ is strongly dense in $\pi^{\mathrm{cpl}}(\mathfrak{A}^{\mathrm{cpl}})$. Indeed, if

$$A = \sum_1^N \pi^{\mathrm{cpl}}(W(x_i^{\mathrm{cpl}})) \in \pi^{\mathrm{cpl}}(\mathfrak{A}^{\mathrm{cpl}})$$

and $x_{i,n} \in \mathcal{X}$ with $x_i \to x_i^{\mathrm{cpl}}$ for η, we obtain that $A_n = \sum_1^N \lambda_i \pi(W(x_{i,n}))$ is bounded by $\sum_1^N |\lambda_i|$ and that $A_n \to A$ strongly on the dense subspace $\pi(\mathfrak{A})\Omega$, and hence on $\mathcal{H}$.

From this fact we see that a closed subspace $\mathcal{K} \subset \mathcal{H}$ is invariant under $\pi(\mathfrak{A})$ iff it is invariant under $\pi^{\mathrm{cpl}}(\mathfrak{A}^{\mathrm{cpl}})$, hence ω is pure iff ω^{cpl} is pure. The statement of the proposition is now proved for example in [**DG**, Theorem 17.13]. □

There is an alternative characterization of pure quasi-free states, due to Kay and Wald [**KW**, eq. (3.34)] which is sometimes very useful.

PROPOSITION 4.9.2. *A quasi-free state on* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ *with covariance* η *is pure iff*

$$x\cdot\eta x=\sup_{x_1\neq 0}\frac{1}{4}\frac{|x\cdot\sigma x_1|^2}{x_1\cdot\eta x_1},\quad x\in\mathcal{X}. \tag{4.35}$$

Proof. It is easy to see that (4.35) on $\mathcal{X}$ is equivalent to (4.35) on $\mathcal{X}^{\mathrm{cpl}}$, so we can assume that $\mathcal{X}$ is complete for η. Note also that from Proposition 4.7.1 (3) $x\cdot\eta x$ is an upper bound of the rhs in (4.35).

If ω is pure we have $2\eta=\sigma\mathrm{j}$ by Proposition 4.9.1, hence $x\cdot\eta\mathrm{j}x=\frac{1}{2}x\cdot\eta x$, which implies (4.35). Let us now prove the converse implication.

Let $c\in L_{\mathrm{a}}(\mathcal{X})$ with $\|c\|\leq 1$ and $\sigma=2\eta c$, as in the beginning of Section 4.8. Note that $\operatorname{Ker}c=\{0\}$ by (4.35). Performing the polar decomposition of c, see e.g. [**DG**, Proposition 2.84], we can write $c=u|c|=|c|u$, where $u\in O(\mathcal{Y},\eta)$ and $u^2=-\mathbb{1}$. Let us check that $|c|=\mathbb{1}$, which will prove that ω is pure. If $|c|\neq\mathbb{1}$, then there exist $\delta\in[0,1[$ and $x\neq 0$ with $x=\mathbb{1}_{[0,\delta]}(|c|)x$, and hence, by Cauchy-Schwarz

$$\big|x\cdot\sigma x_1\big|=2\big||c|x\cdot\eta ux_1\big|\leq 2(|c|x\cdot\eta|c|x)^{\frac{1}{2}}(ux_1\cdot\eta ux_1)^{\frac{1}{2}}=2\delta(x\cdot\eta x)^{\frac{1}{2}}(x_1\cdot\eta x_1)^{\frac{1}{2}},$$

which contradicts (4.35). □

4.9.2. Pure quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},q)$**.** Let us now translate the above results in the case of Hermitian spaces.

Note that Proposition 4.7.6 (2) implies that $\operatorname{Ker}(\lambda^+{+}\lambda^-)=\{0\}$, hence $\|y\|_\omega^2:=\overline{y}\cdot\lambda^+y+\overline{y}\cdot\lambda^-y$ is a Hilbert norm on $\mathcal{Y}$. Denoting by $\mathcal{Y}^{\mathrm{cpl}}$ the completion of $\mathcal{Y}$ for $\|\cdot\|_\omega$, the Hermitian forms $q,\lambda^\pm$ extend uniquely to $q^{\mathrm{cpl}},\lambda^{\pm,\mathrm{cpl}}$ on $\mathcal{Y}^{\mathrm{cpl}}$, and ω extends uniquely to a state ω^{cpl} on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}^{\mathrm{cpl}},q^{\mathrm{cpl}})$. As in the real case, q^{cpl} may be degenerate on $\mathcal{Y}^{\mathrm{cpl}}$.

If $\mathcal{Y}_1\subset\mathcal{Y}^{\mathrm{cpl}}$ with $\mathcal{Y}\subset\mathcal{Y}_1$ densely for $\|\cdot\|_\omega$, then we also obtain unique objects $q_1,\lambda_1^\pm,\omega_1$ that extend $q,\lambda^\pm,\omega$.

The next proposition is the version of Proposition 4.9.1 in the charged case.

PROPOSITION 4.9.3. *A gauge invariant quasi-free state* ω *is pure on* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},q)$ *iff there exists* $\mathcal{Y}_1\subset\mathcal{Y}^{\mathrm{cpl}}$ *with* $\mathcal{Y}\subset\mathcal{Y}_1$ *densely for* $\|\cdot\|_\omega$ *and projections* $c_1^\pm\in L(\mathcal{Y}_1)$ *such that*

$$c_1^++c_1^-=\mathbb{1},\quad \lambda_1^\pm=\pm q_1\circ c_1^\pm. \tag{4.36}$$

Moreover (4.36) *implies that* $c_1^{\pm *}q_1c_1^\mp=0$.

Note that (4.36) implies that q_1 is non-degenerate on $\mathcal{Y}_1$.

Proof. Since $\lambda_1^\pm=\lambda_1^{\pm *}$, we obtain from (4.36) that

$$q_1c_1^\pm=c_1^{\pm *}q_1=c_1^{\pm *}q_1c_1^\pm=c_1^{\pm *}q_1(c_1^++c_1^-),$$

which proves the second claim of the proposition.

(1) Let us now prove the first claim of the proposition if $\mathcal{Y}$ is complete for $\|\cdot\|_\omega$, in which case $\mathcal{Y}_1=\mathcal{Y}$. Recall that j is the complex structure on $\mathcal{Y}$. The real pre-symplectic space $(\mathcal{X},\sigma)$ for $\mathcal{X}=\mathcal{Y}_{\mathbb{R}}$, $\sigma=\operatorname{Im}q$ is then complete for the norm $(x\cdot\eta x)^{\frac{1}{2}}$ and $\eta=\operatorname{Re}(\lambda^\pm\mp\frac{1}{2}q)=\frac{1}{2}\operatorname{Re}(\lambda^++\lambda^-)$.

By Proposition 4.9.1, ω is pure iff there exists an anti-involution j_1 with $2\eta=(\operatorname{Im}q)\mathrm{j}_1$ or equivalently $2\eta\mathrm{j}_1=-(\operatorname{Im}q)$. Since ω is gauge invariant, we have $\mathrm{j}\in sp(\mathcal{X},\operatorname{Im}q)\cap o(\mathcal{X},\eta)$ (see Lemma 4.7.3), hence

$$2\eta\mathrm{j}_1\mathrm{j}=-(\operatorname{Im}q)\mathrm{j}=\mathrm{j}\operatorname{Im}q=-2\mathrm{j}\eta\mathrm{j}_1=2\eta\mathrm{j}\mathrm{j}_1,$$

so $[\mathrm{j},\mathrm{j}_1]=0$, i.e. j_1 is $\mathbb{C}$-linear on $\mathcal{Y}$. Since we know that $\mathrm{j}_1\in Sp(\mathcal{X},\operatorname{Im}q)$ this implies that $\mathrm{j}_1\in U(\mathcal{Y},q)$. Moreover, since $\eta=\operatorname{Re}(\lambda^+-\frac{1}{2}q)$, we have $\operatorname{Re}(2\lambda^+-q)=(\operatorname{Im}q)\mathrm{j}_1$, which using that j_1 is $\mathbb{C}$- linear and λ^+,q are sesquilinear yields $2\lambda^+-q=$

$-q\mathrm{j}\mathrm{j}_1$. We now set $\kappa = -\mathrm{j}\mathrm{j}_1$ so that $\kappa^2 = \mathbb{1}$ and $\kappa \in U(\mathcal{Y}, q)$, $\lambda^+ = \frac{1}{2}(q(\mathbb{1} + \kappa))$. Setting now $c^\pm = \frac{1}{2}(\mathbb{1} + \kappa)$, we see that $c^\pm$ are projections with $c^+ + c^- = \mathbb{1}$, $\lambda^\pm = \pm qc^\pm$. From $\kappa^* q \kappa = q$ we obtain that $c^{\pm *} q c^\mp = 0$, which completes the proof of $\Longrightarrow$.

To prove the implication $\Longleftarrow$, assume that (4.36) holds for $\mathcal{Y}_1 = \mathcal{Y}$ and set $\mathrm{j}_1 = \mathrm{j}(c^+ - c^-)$ so that $\mathrm{j}_1 \in U(\mathcal{Y}, q) \subset Sp(\mathcal{X}, \operatorname{Im} q)$ is an anti-involution. We have $2\lambda^+ - q = q(c^+ - c^-) = -q\mathrm{j}\mathrm{j}_1 = -\mathrm{i}q\mathrm{j}_1$ hence $2\eta = 2\mathrm{Re}(\lambda^+ - q) = (\operatorname{Im} q)\mathrm{j}_1$.

(2) Let us now prove the proposition in the general case. We use the notation in the proof of Proposition 4.9.1 and set additionally $\mathfrak{A}_1 = \mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{Y}_{1,\mathbb{R}}, \operatorname{Re} q_1)$, and $(\mathcal{H}_1, \pi_1, \Omega_1)$ the associated GNS triple. The same argument as in the proof of Proposition 4.9.1 shows then that ω is pure iff ω_1 is pure iff ω^{cpl} is pure. Now the proof of $\Longrightarrow$ follows from (1) by taking $\mathcal{Y}_1 = \mathcal{Y}^{\mathrm{cpl}}$.

Conversely, if (4.36) holds for some space $\mathcal{Y}_1$, then an easy computation shows that as identities on $L(\mathcal{Y}_1, \mathcal{Y}_1^*)$, one has

$$c_1^{\pm *} \lambda_1^\pm c_1^\pm = \lambda_1^\pm, \quad c_1^{\pm *} \lambda_1^\mp c_1^\pm = 0,$$

hence $c_1^\pm$ are bounded for $\|\cdot\|_\omega$. Therefore, they extend to projections on $\mathcal{Y}^{\mathrm{cpl}}$ satisfying (4.36). This implies that ω^{cpl} is pure, hence ω is pure. □

Finally let us prove the analog of Proposition 4.9.2 in the charged case.

Proposition 4.9.4. *A gauge invariant quasi-free state ω with complex covariances $\lambda^\pm$ is pure iff*

$$\overline{y} \cdot (\lambda^+ + \lambda^-) y = \sup_{y_1 \in \mathcal{Y}, y_1 \neq 0} \frac{|\overline{y} \cdot q y_1|^2}{\overline{y}_1 \cdot (\lambda^+ + \lambda^-) y_1}, \quad \forall y \in \mathcal{Y}. \tag{4.37}$$

Proof. Let us set as before $(\mathcal{X}, \sigma) = (\mathcal{Y}_{\mathbb{R}}, \operatorname{Im} q)$ and let η be the real covariance of ω. By Proposition 4.9.2 ω is pure iff

$$y \cdot \eta y_1 = \frac{1}{4} \sup_{y_1 \neq 0} \frac{|y \cdot \operatorname{Im} q y_1|^2}{y_1 \cdot \eta y_1}, \quad y \in \mathcal{Y}.$$

Since $\eta = \frac{1}{2}\mathrm{Re}(\lambda^+ + \lambda^-)$ and q is sesquilinear, this is equivalent to (4.37). □

4.9.3. The GNS representation of pure quasi-free states. The GNS representation of a pure quasi-free state is particularly simple, being a Fock representation. In fact with the notations in Section 4.8 we have $|c| = 1$ and $\sigma = -2\eta\mathrm{j}$.

Set

$$(x_1|x_2)_{\mathrm{F}} := x_1 \cdot \eta x_2 + \frac{\mathrm{i}}{2} x_1 \cdot \sigma x_2, \tag{4.38}$$

and $\mathcal{X}_{\mathrm{F}} := (\mathcal{X}, \mathrm{j}, (\cdot|\cdot)_{\mathrm{F}})$ as a complex Hilbert space. Then the GNS representation of ω is $(\mathcal{H}_{\mathrm{F}}, \pi_{\mathrm{F}}, \Omega_{\mathrm{F}})$, with

$$\mathcal{H}_{\mathrm{F}} = \Gamma_{\mathrm{s}}(\mathcal{X}_{\mathrm{F}}), \quad \pi_{\mathrm{F}} \phi(x) = \phi_{\mathrm{F}}(x), \quad \Omega_{\mathrm{F}} = \Omega_{\mathrm{vac}}.$$

Let us rephrase this in the complex case, where $(\mathcal{Y}, q)$ is a Hermitian space and ω a gauge invariant quasi-free state with complex covariances $\lambda^\pm$. We have, by (4.23),

$$2\eta = \mathrm{Re}(\lambda^+ + \lambda^-), \ \sigma = \operatorname{Im}(\lambda^+ - \lambda^-) = -\mathrm{Re}((\lambda^+ - \lambda^-)\mathrm{i}). \tag{4.39}$$

which yields by an easy computation as in (4.33)

$$2(y_1|y_2)_{\mathrm{F}} = \overline{y}_1 \cdot \lambda^+ y_2 + \overline{y}_2 \cdot \lambda^- y_1. \tag{4.40}$$

Recall that the Hilbert space $\mathcal{Y}^{\mathrm{cpl}}$ was introduced in Subsection 4.9.2. We set $\mathrm{j}_1 = \mathrm{j}(c^+ - c^-)$, and $\mathcal{Y}_{\mathrm{F}} := (\mathcal{Y}^{\mathrm{cpl}}, \mathrm{j}_1, (\cdot|\cdot)_{\mathrm{F}})$, which is a complex Hilbert space. The GNS representation of ω is $(\mathcal{H}_{\mathrm{F}}, \pi_{\mathrm{F}}, \Omega_{\mathrm{F}})$ with

$$\mathcal{H}_{\mathrm{F}} = \Gamma_{\mathrm{s}}(\mathcal{Y}_{\mathrm{F}}), \quad \pi_{\mathrm{F}} \psi^*(y) = a_{\mathrm{F}}^*(c^+ y) + a_{\mathrm{F}}(c^- y), \quad \Omega_{\mathrm{F}} = \Omega_{\mathrm{vac}}.$$

Note that the sesquilinear forms $\lambda^{\pm}$ extend continuously to $\mathcal{Y}_{\rm F}$ (as $\mathbb{R}$-bilinear forms).

4.9.4. The Reeh-Schlieder property for quasi-free states. Let ω be a pure quasi-free state on $\mathrm{CCR}^{\rm pol}(\mathcal{X},\sigma)$. If $\mathcal{X}_1\subset\mathcal{X}$ is a (real) vector subspace, then by Theorem 4.8.1 we know that $\mathrm{Vect}\{W_{\rm F}(x)\Omega_{\rm F}\,:\,x\in\mathcal{X}_1\}$ is dense in the GNS Hilbert space $\mathcal{H}_{\rm F}$ iff $\mathbb{C}\mathcal{X}_1$ is dense in the Hilbert space $\mathcal{X}_{\rm F}$ introduced above.

It is convenient to have a version of this result in the complex case. We fix a space $(\mathcal{Y},q)$ and a *pure* gauge invariant quasi-free state ω on $\mathrm{CCR}^{\rm pol}(\mathcal{Y},q)$, with complex covariances $\lambda^{\pm}$. Let us denote by j the charge complex structure of $\mathcal{Y}$.

Proposition 4.9.5. *Let $\mathcal{Y}_1\subset\mathcal{Y}$ be a complex vector subspace of $\mathcal{Y}$. Then* $\mathrm{Vect}\{W_{\rm F}(y)\Omega_{\rm F}:y\in\mathcal{Y}_1\}$ *is dense in the* GNS *Hilbert space $\mathcal{H}_{\rm F}$ iff*

$$\overline{y}\cdot\lambda^{+}y_1=\overline{y}\cdot\lambda^{-}y_1=0\ \forall\ y_1\in\mathcal{Y}_1\Longrightarrow y=0,\ \textit{for } y\in\mathcal{Y}^{\rm cpl}. \tag{4.41}$$

Proof. By (4.38) and Theorem 4.8.1, $\mathrm{Vect}\{W_{\rm F}(y)\Omega_{\rm F}:y\in\mathcal{Y}_1\}$ is dense in $\mathcal{H}_{\rm F}$ iff

$$y\cdot\eta y_1=y\cdot\sigma y_1=0\ \forall\ y_1\in\mathcal{Y}_1\Longrightarrow y=0. \tag{4.42}$$

Next we use (4.39) and the fact that $\mathrm{j}\mathcal{Y}_1=\mathcal{Y}_1$ to obtain that (4.42) is equivalent to (4.41). □

4.10. Examples

4.10.1. The vacuum state for real Klein-Gordon fields. We can take as real symplectic space $(\mathcal{X},\sigma)$ either the space $(C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),\sigma)$ with σ defined in (2.16), or the space $(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{R})}{PC_0^\infty(\mathbb{R}^n;\mathbb{R})},(\cdot|G\cdot)_{\mathbb{R}^n})$.

If we take the first version we obtain from (3.10) that

$$f\cdot\eta g=\frac{1}{2}(f_0|\epsilon g_0)_{L^2(\mathbb{R}^d)}+\frac{1}{2}(f_1|\epsilon^{-1}g_1)_{L^2(\mathbb{R}^d)},\quad f,g\in(C_0^\infty(\mathbb{R}^d;\mathbb{R}^2),\sigma). \tag{4.43}$$

In the second version, we obtain from (3.14) and (3.15) that

$$u\cdot\eta v=\int_{\mathbb{R}^n\times\mathbb{R}^n}u(x)\eta(x,x')v(x')dxdx',\quad u,v\in C_0^\infty(\mathbb{R}^n;\mathbb{R})$$

where

$$\eta(x,x')=(2\pi)^{-n}\int_{\mathbb{R}^d}\frac{1}{2\epsilon(\mathrm{k})}\cos((t-t')\epsilon(\mathrm{k}))\mathrm{e}^{\mathrm{i}\mathrm{k}\cdot(\mathrm{x}-\mathrm{x}')}d\mathrm{k}. \tag{4.44}$$

4.10.2. The vacuum state for complex Klein-Gordon fields. It is more convenient to consider complex solutions of the Klein-Gordon equation. We take as Hermitian space $(\mathcal{Y},q)$ either $(C_0^\infty(\mathbb{R}^d;\mathbb{C}^2),q)$ with q defined in (2.21), or $(\frac{C_0^\infty(\mathbb{R}^n;\mathbb{C})}{PC_0^\infty(\mathbb{R}^n;\mathbb{C})},(\cdot|\mathrm{i}G\cdot)_{\mathbb{R}^n})$, see Theorem 2.4.1.

In the first case the complex covariances $\lambda^{\pm}$ of the vacuum state $\omega_{\rm vac}$ are given by

$$\lambda^{\pm}=\frac{1}{2}\begin{pmatrix}\epsilon & \pm\mathbb{1}\\ \pm\mathbb{1} & \epsilon^{-1}\end{pmatrix}, \tag{4.45}$$

where we identify sesquilinear forms with operators using the scalar product on $L^2(\mathbb{R}^d;\mathbb{C}^2)$. The projections $c^{\pm}$ in Proposition 4.9.3 equal

$$c^{\pm}=\frac{1}{2}\begin{pmatrix}\mathbb{1} & \pm\epsilon^{-1}\\ \pm\epsilon & \mathbb{1}\end{pmatrix}. \tag{4.46}$$

Note that

$$U_0(t)c^{\pm}f=\mathrm{e}^{\pm\mathrm{i}\epsilon t}(f_0\pm\epsilon^{-1}f_1),$$

so $c^{\pm}$ are the projections on the spaces of Cauchy data of solutions with *positive/negative energy.*

If we take the second version and denote by

$$\Lambda^{\pm} = (\varrho_0 \circ G)^* \lambda^{\pm} (\varrho_0 \circ G)$$

the corresponding complex covariances, their distributional kernels are given by

$$\Lambda^{\pm}(x, x') = (2\pi)^{-n} \int \frac{1}{2\epsilon(\mathrm{k})} \mathrm{e}^{\pm \mathrm{i}(t-t')\epsilon(\mathrm{k}) + \mathrm{i}\mathrm{k}\cdot(\mathrm{x}-\mathrm{x}')} d\mathrm{k}. \tag{4.47}$$

4.10.3. Vacuum and kms states for abstract Klein-Gordon equations. Let us fix a complex Hilbert space $\mathfrak{h}$ and $\epsilon^2 > 0$ a selfadjoint operator on $\mathfrak{h}$. Let us consider the following abstract Klein-Gordon equation:

$$\partial_t^2 \phi(t) + \epsilon^2 \phi(t) = 0, \quad \phi : \mathbb{R} \to \mathfrak{h}. \tag{4.48}$$

The main example is the Klein-Gordon equation on an *ultra-static* spacetime $M = \mathbb{R} \times S$, where (S, h) is a complete Riemannian manifold and M is equipped with the Lorentzian metric $g = -dt^2 + h_{ij}(\mathrm{x}) d\mathrm{x}^i d\mathrm{x}^j$. We take then $\mathfrak{h} = L^2(\Sigma, dVol_h)$ and $\epsilon^2 = -\Delta_h + m^2$, where $-\Delta_h$ is the Laplace-Beltrami operator on (Σ, h).

We take as Hermitian space

$$\mathcal{Y} = \epsilon^{-\frac{1}{2}} \mathfrak{h} \oplus \epsilon^{\frac{1}{2}} \mathfrak{h}, \quad \overline{f} \cdot q f = (f_1 | f_0)_{\mathfrak{h}} + (f_0 | f_1)_{\mathfrak{h}}.$$

The *vacuum state* ω_{vac} is now defined by the complex covariances $\lambda^{\pm}$ in (4.45), where we again identify sesquilinear forms and operators using the scalar product on $\mathfrak{h} \oplus \mathfrak{h}$.

Another natural quasi-free state is the *kms state* ω_β at temperature β^{-1}, given by the covariances

$$\lambda_\beta^{\pm} = \frac{1}{2} \begin{pmatrix} \epsilon \mathrm{th}(\beta\epsilon/2) & \pm \mathbb{1} \\ \pm \mathbb{1} & \epsilon^{-1} \mathrm{th}(\beta\epsilon/2) \end{pmatrix}, \tag{4.49}$$

which is not a pure state. ω_{vac} resp. ω_β, is a ground state, resp. a β-KMS state for the dynamics $\{r_s\}_{s \in \mathbb{R}}$ defined by $r_s \phi(\cdot) = \phi(\cdot + s)$, for ϕ solution of (4.48). We refer the reader to Section 9.1 for a general discussion of KMS states.

CHAPTER 5

Free Klein-Gordon fields on curved spacetimes

In this chapter we describe some well-known results about Klein-Gordon equations on Lorentzian manifolds. An important notion is the *causal structure* obtained from a Lorentzian metric, which leads to the notion of *globally hyperbolic spacetimes*, originally introduced by Leray [**Le**].

Globally hyperbolic spacetimes are Lorentzian manifolds which admit a *Cauchy surface*, i.e. a hypersurface intersected only once by each inextensible causal curve.

On a globally hyperbolic spacetime M, one can pose and globally solve the *Cauchy problem* for the Klein-Gordon operators P associated to the metric g. Equivalently one can uniquely solve the inhomogeneous Klein-Gordon equation with *support conditions*, i.e. introduce the *retarded/advanced inverses* $G_{\mathrm{ret/adv}}$ for P.

The *causal propagator* $G = G_{\mathrm{ret}} - G_{\mathrm{adv}}$ is anti-symmetric and hence can be used to equip the space of test functions on the spacetime M with the structure of a pre-symplectic space, see Lichnerowicz [**Li1**] and Dimock [**Di1**]. If one fixes a Cauchy surface Σ, one can equivalently use the symplectic space of Cauchy data on Σ, i.e. of pairs of compactly supported smooth functions on Σ. This is particularly important for the construction of states for quantized Klein-Gordon fields, see Chapter 6.

5.1. Background

We now collect some background material on vector bundles and connections on them. Most of it will be used only in Chapter 17 and can be skipped in first reading.

5.1.1. Fiber bundles. Let E, M be two smooth manifolds and $\pi : E \to M$ surjective with $D_e\pi$ surjective for each $e \in E$. The set $E_x = \pi^{-1}(\{x\})$ is called the *fiber* over $x \in M$. Let F be another smooth manifold. $E \xrightarrow{\pi} M$ is a *fiber bundle* with *typical fiber* F if there exists an open covering $\{U_i\}_{i\in I}$ of M such that for each U_i there exists $\phi_i : \pi^{-1}(U_i) \xrightarrow{\sim} U_i \times F$ such that

$$\pi_M \circ \phi_i = \pi \quad \text{on } \pi^{-1}(U_i).$$

The maps ϕ_i are called *local trivializations* of the bundle $E \xrightarrow{\pi} M$. The collection $\{(U_i, \phi_i)\}_{i\in I}$ is called a *bundle atlas* for the bundle $E \xrightarrow{\pi} M$. For U_i, U_j with $U_{ij} := U_i \cap U_j \neq \emptyset$, we have

$$\phi_i \circ \phi_j^{-1}(x, f) = (x, t_{ij}(x)(f)),$$

where the maps $t_{ij} : U_{ij} \to Aut(F)$ are called *transition maps*. One has

$$t_{ii}(x) = Id, \quad t_{ik}(x) = t_{ij}(x) \circ t_{jk}(x), \quad x \in U_i \cap U_j \cap U_k. \tag{5.1}$$

A fiber bundle $E \xrightarrow{\pi} M$ can be reconstructed from a covering $\{U_i\}_{i\in I}$ of M and from a set of transition maps satisfying (5.1).

5.1.2. Morphisms of bundles. If $E \xrightarrow{\pi} M$ and $E' \xrightarrow{\pi'} M$ are two fiber bundles with typical fibers F and F', a smooth map $\chi : E \to E'$ is a *bundle morphism* if $\pi' \circ \chi = \pi$. If t_{ij}, resp. t'_{ij} are the transition maps of E, resp E', then there exists $\chi_i : U_i \to Hom(F, F')$ such that

$$t'_{ij} \circ \chi_j = \chi_i \circ t_{ij} \text{ on } U_{ij}. \tag{5.2}$$

A fiber bundle $E \xrightarrow{\pi} M$ is trivial if there exists a bundle isomorphism $\chi : E \to M \times F$. By (5.2), this is the case iff there exists $\chi_i : U_i \to Aut(F)$ such that

$$t_{ij} = \chi_i^{-1} \circ \chi_j \text{ on } U_{ij}. \tag{5.3}$$

5.1.3. Sections of a bundle. A (smooth) section of a bundle $E \xrightarrow{\pi} M$ is a smooth map $f : M \to E$ such that $\pi \circ f = Id$. The space of smooth sections of $E \xrightarrow{\pi} M$ will be denoted (somewhat improperly) by $C^\infty(M; E)$.

5.1.4. Fiber bundles with structure group G. Let $E \xrightarrow{\pi} M$ a fiber bundle and G a group with an injective morphism $\rho : G \to Aut(F)$, where F is the typical fiber of E. One says that $E \xrightarrow{\pi} M$ has G as *structure group* and one writes $G \to E \xrightarrow{\pi} M$ if for all compatible i, j one has

$$t_{ij}(x) = \rho(g_{ij}(x)), \text{ with } g_{ij} : U_{ij} \longrightarrow G.$$

The maps g_{ij} satisfy of course (5.1).

5.1.5. Principal bundles. There is a canonical injective morphism $\rho : G \to Aut(G)$ given by *left* multiplication. A bundle $P \xrightarrow{\pi} M$ with G as fiber and structure group for the above action is called a *G-principal bundle*. Its transition maps are given by maps

$$g_{ij} : U_{ij} \longrightarrow G \subset Aut(G).$$

Equivalently, a bundle $P \xrightarrow{\pi} M$ is a G-principal bundle if there is a *right action* of G on P, which preserves the fibers and acts freely and transitively on the fibers. It is known that a principal bundle is trivial iff it has a global section.

5.1.6. Vector bundles. Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. A bundle $E \xrightarrow{\pi} M$ with typical fiber $\mathbb{K}^n$ is called a *vector bundle* of rank n if E_x is an n-dimensional vector space over $\mathbb{K}$ for each $x \in M$ and the maps

$$\phi_{i,x} = \pi_F \circ \phi_{i|E_x} : E_x \to \mathbb{K}^n, \quad x \in U_i$$

are $\mathbb{K}$-linear. If t_{ij} are the transition functions of E one has $t_{ij} : U_{ij} \to GL_n(\mathbb{K})$. If each fiber E_x is oriented and the maps $\phi_{i,x} : E_x \to \mathbb{K}^n$ are orientation preserving, the vector bundle $E \xrightarrow{\pi} M$ is said to be *oriented*, and in this case the transition maps $t_{ij}(x)$ take values in $GL_n^+(\mathbb{K})$.

If $E \xrightarrow{\pi} M$ is a vector bundle, we denote by $C^\infty(M; E)$, resp. $C_0^\infty(M; E)$, the space of smooth resp. smooth compactly supported, sections of E.

Similarly, one denotes by $\mathcal{D}'(M; E)$, $\mathcal{E}'(M; E)$ the space of distributional, resp., compactly supported distributional sections of E.

If (M, g) is a spacetime, one denotes by $C_{\mathrm{sc}}^\infty(M; E)$ the space of smooth *space-compact* sections of E, see Subsection 5.2.6 for terminology.

5.1.7. Tangent and cotangent bundles. If M is a smooth manifold of dimension n, its *tangent bundle* $TM \xrightarrow{\pi} M$ is the vector bundle with fiber $\mathbb{R}^n$ and transition maps

$$U_{ij} \ni x \mapsto D_x\chi_{ij} \in GL_n(\mathbb{R}),$$

where $\{(U_i, \chi_i)\}_{i\in I}$ is an atlas of M and $\chi_{ij} = \chi_i \circ \chi_j^{-1}$. Likewise its *cotangent bundle* $T^*M \xrightarrow{\pi} M$ is the vector bundle with fiber $\mathbb{R}^n$ and transition maps

$$U_{ij} \ni x \mapsto ({}^tD_x\chi_{ij})^{-1} \in GL_n(\mathbb{R}).$$

We denote by $\wedge^p(M)$ the bundle of p-forms on M and set

$$\wedge(M) = \bigoplus_{p=0}^{n} \wedge^p(M).$$

M is *orientable* if $\wedge^n(M)$ admits a non-zero global section. If this is the case the transition maps t_{ij} of TM can be chosen so that $\det t_{ij} > 0$ on U_{ij}.

5.1.8. Metric vector bundles. A vector bundle $E \xrightarrow{\pi} M$ is a *metric vector bundle* (of signature (q, p)) if each fiber E_x is equipped with a non-degenerate scalar product h_x and

$$\phi_{i,x} : (E_x, h_x) \longrightarrow \mathbb{R}^{q,p} \text{ is orthogonal for } x \in U_i,$$

where $\mathbb{R}^{q,p}$ is $\mathbb{R}^{q+p}$ with the canonical scalar product $-\sum_{i=1}^{q} x_i^2 + \sum_{i=q+1}^{p+q} x_i^2$.

5.1.9. Dual vector bundle. Let $E \xrightarrow{\pi} M$ a vector bundle of rank n. The *dual bundle* $E' \xrightarrow{\pi} M$ is defined by the fibers $E'_x = (E_x)'$ and the transition maps $(t_{ij}^{-1})'$.

5.1.10. Bundle of frames. Let $E \xrightarrow{\pi} M$ a vector bundle of rank n. We can associate to it the *bundle of frames* of E, denoted by $Fr(E) \xrightarrow{\pi} M$ and defined as follows: one sets

$$Fr(E) = \bigsqcup_{x\in M} Fr(E_x),$$

where $Fr(V)$ is the set of ordered bases (i.e. frames) of the vector space V, i.e. of linear isomorphisms $\mathcal{F} : \mathbb{K}^n \xrightarrow{\sim} E_x$. The transition functions of $Fr(E)$ are

$$T_{ij}(x) : GL_n(\mathbb{K}) \in A \longmapsto t_{ij}(x) \circ A \in GL_n(\mathbb{K}), \quad x \in U_{ij},$$

where $t_{ij} : U_{ij} \to GL_n(\mathbb{K})$ are the transition functions of E. The bundle $Fr(E) \xrightarrow{\pi} M$ is a $GL_n(\mathbb{K})$-principal bundle.

5.1.11. The bundle $End(E)$. Let $E \xrightarrow{\pi} M$ a vector bundle of rank n. One defines the vector bundle $End(E) \xrightarrow{\pi} M$ with fibers $End(E)_x = End(E_x)$ and transition maps $A \to t_{ij}(x) \circ A \circ t_{ij}^{-1}(x)$, $x \in M$, $A \in End(\mathbb{K}^n)$.

5.1.12. The bundle $E_1 \boxtimes E_2$. Let $E_i \xrightarrow{\pi} M_i$ be vector bundles of rank n_i, $i = 1, 2$. One can form the vector bundle $E_1 \boxtimes E_2 \xrightarrow{\pi} M_1 \times M_2$, with fibers $E_{1,x_1} \otimes E_{2,x_2}$ over (x_1, x_2). If $\{U_{i,j_i}\}_{j_i\in I_i}$ and t_{i,j_i,k_i} are coverings and transition maps for $E_i \xrightarrow{\pi} M_i$, then one takes $\{U_{1,j_1} \times U_{2,j_2}\}_{(j_1,j_2)\in I_1\times I_2}$ as covering of $M_1 \times M_2$ and $t_{1,j_1,k_1} \otimes t_{2,j_2,k_2}$ as transition maps.

5.1.13. The bundle $End(E, E^*)$. If $E \xrightarrow{\pi} M$ is a complex vector bundle of rank n, the bundle $End(E, E^*) \xrightarrow{\pi} M$ is the bundle with fibers $End(E, E^*)_x = End(E_x, E_x^*)$ and transition maps $A \to t_{ij}(x)^* \circ A \circ t_{ij}(x)$, $x \in M$, $A \in End(\mathbb{C}^n, \mathbb{C}^{n*})$.

A vector bundle E equipped with a smooth section λ of $End(E, E^*)$ such that $\lambda(x)$ is a non-degenerate Hermitian form on E_x for all $x \in M$ is called a *Hermitian vector bundle*.

5.1.14. Connections on vector bundles. Let E a complex vector bundle over M. Note that $C^\infty(M;E)$ is a $C^\infty(M)$ module. A *connection* ∇ on E is a bilinear map

$$\nabla : C^\infty(M;TM) \times C^\infty(M;E) \longrightarrow C^\infty(M;E)$$

such that

$$\nabla_X(f\varphi) = X(f)\varphi + f\nabla_X\varphi,$$
$$\nabla_{fX}\varphi = f\nabla_X\varphi, \quad f \in C^\infty(M),\ X \in C^\infty(M;TM),\ \varphi \in C^\infty(M;E).$$

If g is a metric on M, there exists a unique connection on TM, called the *Levi-Civita connection*, denoted by ∇^g or often simply by ∇, such that

$$\begin{aligned} &X(X_1 \cdot gX_2) = \nabla_X X_1 \cdot gX_2 + X_1 \cdot g\nabla_X X_2, \quad X, X_1, X_2 \in C^\infty(M;TM), \\ &\nabla_{X_1}X_2 - \nabla_{X_2}X_1 = [X_1, X_2], \quad X_1, X_2 \in C^\infty(M;TM). \end{aligned} \tag{5.4}$$

5.1.15. Stokes formula. Let M be a smooth n-dimensional manifold, $\Sigma \subset M$ a smooth hypersurface, $i : \Sigma \to M$ the canonical injection, and $i^* : \wedge(M) \to \wedge(\Sigma)$ the pullback by i.

A vector field X over Σ, i.e. a smooth section of $T_\Sigma M$ is said to be *transverse* to Σ if $T_xM = \mathbb{R}X_x \oplus T_x\Sigma$ for each $x \in \Sigma$. One still denotes by X any of its smooth extensions as a section of TM, supported in a neighborhood of Σ in M.

If $\omega \in C^\infty(M; \wedge^p(M))$, then $X \lrcorner \omega \in C^\infty(M; \wedge^{p-1}(M))$, where $\lrcorner$ denotes the interior product, and one sets:

$$i_X^*\omega := i^*(X \lrcorner \omega) \in C^\infty(\Sigma, \wedge^{p-1}(\Sigma)).$$

One uses the same procedure to pullback *densities* on M to densities on Σ: if $\mu = |\omega|$ for $\omega \in C^\infty(M; \wedge^n(M))$ is a smooth density on M, we set $i_X^*\mu := |i_X^*\omega|$ which is a smooth density on Σ.

In local coordinates $(x^1, \ldots, x^n)$, in which $\Sigma = \{x^1 = 0\}$, X is transverse to Σ iff $X^1(0, x^2, \ldots, x^n) \neq 0$, and if $\mu = f dx^1 \cdots dx^n$, then

$$i_X^*\mu = f(0, x^2, \ldots, x^n)|X^1(0, x^2, \ldots, x^n)| dx^2 \cdots dx^n.$$

We will always assume that M is orientable, see Subsection 5.1.7, and fix a smooth, nowhere vanishing n-form $\omega_{\rm or}$ on M.

If $U \subset M$ is an open set such that ∂U is a finite union of smooth hypersurfaces, then one orients ∂U by the $(n-1)$-form $i_X^*\omega_{\rm or}$, where X is an outwards pointing, transverse vector field to ∂U and $i : \partial U \to M$ is the canonical injection. We recall *Stokes' formula*:

$$\int_U d\omega = \int_{\partial U} i^*\omega, \quad \omega \in C^\infty(M; \wedge^{n-1}(M)). \tag{5.5}$$

5.2. Lorentzian manifolds

A *Lorentzian manifold* is a pair (M, g), where M is a smooth n-dimensional manifold and g is a Lorentzian metric on M, i.e. a smooth map $M \ni x \mapsto g(x)$, where $g(x) \in L_{\rm s}(T_xM, T_x'M)$ has signature $(1, n-1)$. It is customary to write g as $g_{\mu\nu}(x)dx^\mu dx^\nu$ or $g(x)dx^2$ and to denote the inverse metric $g^{-1}(x) \in L_{\rm s}(T_xM', T_xM)$ as $g^{\mu\nu}(x)d\xi_\mu d\xi_\nu$ or $g^{-1}(x)d\xi^2$.

Definition 5.2.1. (1) *A vector $v \in T_xM$ is* time-like *if $v \cdot g(x)v < 0$,* null *if $v \cdot g(x)v = 0$,* causal *if $v \cdot g(x)v \leq 0$, and* space-like *if $v \cdot g(x)v > 0$.*

(2) *Similarly, a vector field v on M is* time-like*, etc., if $v(x)$ is time-like, etc., for each $x \in M$.*

(3) *The cone of time-like, resp. null vectors in T_xM is denoted by $C(x)$, resp. $N(x)$.*

DEFINITION 5.2.2. *A vector subspace $V \subset T_xM$ is* time-like *if it contains both space-like and time-like vectors,* null *if it is tangent to the lightcone $N(x)$, and* space-like *if it contains only space-like vectors.*

LEMMA 5.2.3. *If $V \subset T_xM$ is a vector subspace, one denotes by $V^\perp$ its orthogonal for $g(x)$. Then V is time-like, resp. null, space-like iff $V^\perp$ is space-like, resp. null, time-like.*

We refer to [**Fr**, Lemma 3.1.1] for the proof.
There is a similar terminology for submanifolds $N \subset M$.

DEFINITION 5.2.4. *A submanifold $N \subset M$ is* time-like *resp.* space-like, null *if T_xN is time-like resp. space-like, null for each $x \in N$.*

Null submanifolds are also called *characteristic*.

5.2.1. Volume forms and volume densities. The metric g induces a scalar product $(\cdot|\cdot)_g$ on the fibers $\wedge^p_x(M) = \wedge^p T'_xM$, defined by

$$(u_1 \wedge \cdots \wedge u_p | v_1 \wedge \cdots \wedge v_p)_{g(x)} = \det(u_i \cdot g^{-1}(x) v_j) \quad 1 \leq p \leq n. \tag{5.6}$$

Assuming that M is orientable, one obtains a unique n-form $\Omega_g \in C^\infty(M; \wedge^n M)$, called the *volume form*, such that $(\Omega_g|\Omega_g)_{g(x)} = 1$ for all $x \in M$ and Ω_g is positively oriented. The *volume density* is the 1-density

$$dVol_g := |\Omega_g|.$$

If $(x^1, \ldots, x^n)$ are local coordinates on M such that $dx^1 \wedge \cdots \wedge dx^n$ is positively oriented, then one has:

$$\Omega_g = |g(x)|^{\frac{1}{2}} dx^1 \wedge \cdots \wedge dx^n, \quad dVol_g = |g(x)|^{\frac{1}{2}} dx^1 \cdots dx^n, \tag{5.7}$$

where $|g(x)| = \det(g_{ij}(x))$.

5.2.2. Distributions on M. We denote by $\mathcal{D}'(M)$, resp. $\mathcal{E}'(M)$, the space of distributions on M, resp. compactly supported distributions, see e.g. [**H1**, Section 6.3] for definitions. The topological dual of $C^\infty_0(M)$, resp. $C^\infty(M)$, is the space of *distribution densities*, resp. distribution densities of compact support. One identifies each distribution u with the distribution density $udVol_g$. Setting

$$(u|v)_M := \int_M \overline{u} v \, dVol_g, \tag{5.8}$$

leads to the following natural notation

$$(u|v)_M := \langle \overline{u} \, dVol_g | v \rangle, \quad \text{for } u \in \mathcal{D}'(M), v \in C^\infty_0(M), \tag{5.9}$$

where $\langle \cdot | \cdot \rangle$ is the duality bracket.

5.2.3. Normal vector field. If $\Sigma \subset M$ is a smooth hypersurface which is not null, there is a unique (up to sign) transverse vector field n, which is *normal* and *normalized*, i.e.

$$n(x) \cdot g(x) v = 0, \quad |n(x) \cdot g(x) n(x)| = 1, \quad \forall v \in T_x\Sigma, x \in \Sigma.$$

The induced metric on Σ, $h := i^* g$, is non-degenerate and one has

$$\Omega_h = i^*_n \Omega_g, \quad i^*_X \Omega_g = X^a \cdot n_a \Omega_h, \tag{5.10}$$

if X is a vector field on Σ. This can be easily checked in local coordinates, using (5.7).

5.2.4. Gauss formula. If X is a vector field on M, then

$$\nabla_a X^a \Omega_g = d(X \lrcorner \Omega_g), \tag{5.11}$$

where ∇ is the Levi-Civita connection associated to g, hence Stokes' formula can be rewritten as

$$\int_U \nabla^a X_a dVol_g = \int_{\partial U} i_X^* dVol_g. \tag{5.12}$$

To express the right-hand side of (5.12), we fix a vector field l that is transverse to ∂U and outwards pointing. Let ν be a 1-form on M such that $\operatorname{Ker} \nu = T\partial U$, normalized such that $\nu \cdot l = 1$. It follows that if X is a vector field on M we have

$$X = (\nu \cdot X) l + R, \quad \text{where } R \text{ is tangent to } \partial U.$$

Since R is tangent to ∂U, we have $i^*(R \lrcorner dVol_g) = 0$, hence

$$i_X^* dVol_g = (\nu \cdot X) i_l^* (dVol_g).$$

Thus, we obtain the Gauss formula

$$\int_U \nabla_a X^a dVol_g = \int_{\partial U} \nu_a X^a i_l^* dVol_g. \tag{5.13}$$

Let Σ be one of the connected components of ∂U.

If Σ is given by $\{f = 0\}$ for some function f with $df \neq 0$ on Σ, and if we can complete f near Σ with coordinates $y^1, \dots, y^{n-1}$ such that $df \wedge dy^1 \wedge \cdots \wedge dy^{n-1}$ is direct, with ∂_f pointing outwards, then we take $l = \partial_f$, $\nu = df$ and obtain

$$i_X^*(dVol_g) = X^a \nabla_a f |g|^{\frac{1}{2}} dy^1 \cdots dy^{n-1} \text{ on } \Sigma. \tag{5.14}$$

5.2.5. Non-characteristic boundaries. If Σ is non-characteristic, we can take $l = n$, the outwards pointing normal vector field to Σ. Since $i_n^* dVol_g = dVol_h$ we obtain

$$i_X^* dVol_g = n_a X^a dVol_h \quad \text{on } \Sigma. \tag{5.15}$$

5.2.6. Causal structures. We now recall some notions related to the *causal structure* on M induced by the metric g. All the objects below are of course unchanged under a conformal transformation $g \to c^2 g$ of the metric, where $c \in C^\infty(M)$ is a strictly positive function.

DEFINITION 5.2.5. (1) *A Lorentzian manifold is* time orientable *if it carries a continuous time-like vector field v. Given such a vector field, one denotes by $C_\pm(x)$ the connected component of $C(x)$ such that $\pm v(x) \in C_\pm(x)$.*

(2) *The vectors in $C_\pm(x)$ are called* future/past directed*, and one uses the same terminology for time-like vector fields. Such a continuous choice of $C_\pm(x)$ is called a* time orientation*.*

(3) *A time oriented Lorentzian manifold is called a* spacetime*.*

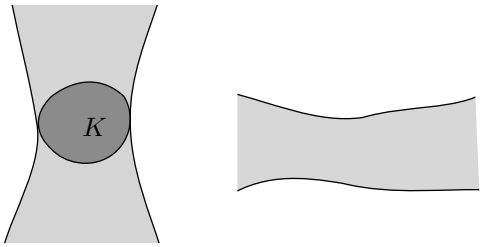
In the sequel, we will always assume that the Lorentzian manifold M is orientable, see Subsection 5.1.6, and by spacetime we will always mean an *orientable spacetime*.

DEFINITION 5.2.6. *Let (M, g) be a spacetime and $\gamma : I \ni s \mapsto x(s) \in M$ a piecewise C^1 curve.*

(1) *γ is* time-like*, resp.* null*,* space-like*,* future/past directed *if all its tangent vectors $x'(s), s \in I$ are so.*

(2) *γ is* inextensible *if no piecewise C^1 reparametrization of γ can be continuously extended beyond its endpoints.*

DEFINITION 5.2.7. (1) *The* time-like *resp.* causal future/past *of $x \in M$, denoted by $I_\pm(x)$, resp. $J_\pm(x)$, is the set of points belonging to time-like, resp. causal future/past directed curves γ starting at x.*
(2) *For $K \subset M$ one sets $I_\pm(K) = \bigcup_{x\in K} I_\pm(x)$, $J_\pm(K) = \bigcup_{x\in K} J_\pm(x)$*
(3) *The* time-like, *resp.* causal shadow *of $K \subset M$ is $I(K) = I_+(K) \cup I_-(K)$, resp. $J(K) = J_+(K) \cup J_-(K)$.*
(4) *Two sets K_1, K_2 are* causally disjoint *if $J(K_1) \cap K_2 = \emptyset$, or, equivalently if $J(K_2) \cap K_1 = \emptyset$.*
(5) *A closed set $A \subset M$ is* space-compact, *resp.* future/past space-compact *if $A \subset J(K)$, resp. $A \subset J_\pm(K)$ for some compact set $K \Subset M$.*
(6) *A closed set $A \subset M$ is* time-compact, *resp.* future/past time compact *if $A \cap J(K)$, resp. $A \cap J_\mp(K)$ is compact for each compact set $K \Subset M$.*



a space-compact set a time-compact set

Fig. 1

Note that if $U \subset M$ is an open subset of the spacetime (M, g), then (U, g) is a spacetime as well. In this case if $K \subset U$, we use the notation $J^U_\pm(K)$, resp. $J^M_\pm(K)$ for the future/past causal shadows of K in U resp. in M.

One says that $U \subset M$ is *causally compatible* if $J^U_\pm(x) = J^M_\pm(x) \cap U$ for each $x \in U$. This is equivalent to the property that a causal curve in M between two points $x, x' \in U$ is entirely contained in U. The same terminology is used for an isometric embedding $i : (M', g') \to (M, g)$. An example of a non-causally compatible domain U in Minkowski spacetime is given in Fig. 2 below.

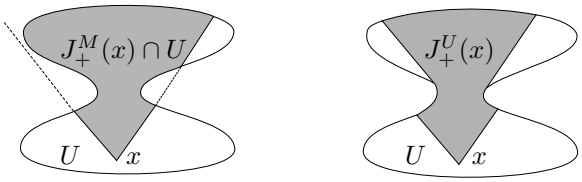


Fig. 2

5.3. Stationary and static spacetimes

5.3.1. Killing vector fields. Let X a smooth vector field on M whose flow $s \mapsto \phi_X(s)$ is complete. X is called a *Killing vector field* for (M, g) if $\phi_X(s)$ are isometries of (M, g), i.e. $\phi_X(s)^*(g) = g$ for $s \in \mathbb{R}$. Equivalently, X should satisfy *Killing's equation*

$$\nabla_a X_b + \nabla_b X_a = 0,$$

where ∇ is the Levi-Civita connection for g.

5.3.2. Stationary spacetimes.

DEFINITION 5.3.1. *The spacetime* (M, g) *is* stationary *if it admits a complete, time-like future directed Killing vector field* X*.*

The standard model of a stationary spacetime is as follows: let (S, h) be a Riemannian manifold , $N \in C^\infty(S)$ with $N > 0$, and $w_i dx^i$ be a smooth 1-form on S. Let $M = \mathbb{R}_t \times S_x$ and

$$g = -N^2(x)dt^2 + (dx^i + w^i(x)dt)h_{ij}(x)(dx^j + w^j(x)dt).$$

Then (M, g) is stationary with Killing vector field ∂_t if $N^2(x) > w_i(x)h^{ij}(x)w_j(x)$, $x \in S$.

It is known, see e.g. [**S2**, Proposition 3.1], that a stationary spacetime which is also *globally hyperbolic* (see Section 5.4) is isometric to such a model.

5.3.3. Static spacetimes. A stationary spacetime (M, g) with Killing vector field X is called *static* if there exists a smooth hypersurface S which is everywhere g-orthogonal to X. The standard model of a static spacetime is the one above for $w_i dx^i = 0$. A static, globally hyperbolic spacetime is isometric to the standard model iff one can choose S to be a Cauchy surface, see [**S2**, Proposition 3.2].

An *ultra-static* space time is a spacetime $M = \mathbb{R} \times S$ with the Lorentzian metric $g = -dt^2 + h(x)dx^2$, where (S, h) is a Riemannian manifold. It is known that (M, g) is globally hyperbolic iff (S, h) is complete, see [**S**, Theorem 3.1], [**Ky1**, Proposition 5.2].

5.4. Globally hyperbolic spacetimes

DEFINITION 5.4.1. *A* Cauchy surface S *is a closed set* $S \subset M$ *which is intersected exactly once by each inextensible time-like curve.*

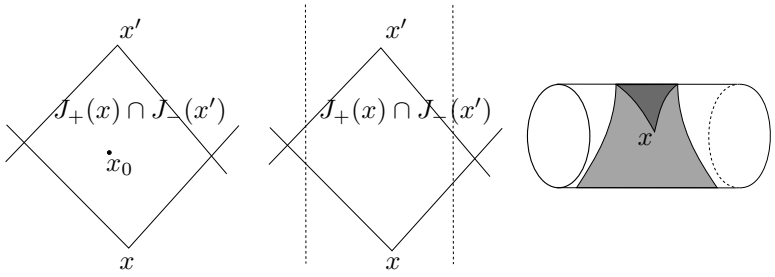
DEFINITION 5.4.2. *A spacetime* (M, g) *is* globally hyperbolic *if the following conditions hold:*

(1) $J_+(x) \cap J_-(x')$ *is compact for all* $x, x' \in M$*,*
(2) M *is* causal*, i.e. there are no closed causal curves in* M*.*

The original definition of global hyperbolicity required the stronger condition of *strong causality*, see e.g. [**BGP**, Definition 1.3.8], [**W1**, Section 8.3]. The fact that the two definitions are equivalent is due to Bernal and Sanchez [**BS3**].

Here are three elementary examples of non-globally hyperbolic spacetimes:

(1) $M = \mathbb{R}^{1,1} \backslash \{x_0\}$: $J_+(x) \cap J_-(x')$ may not be compact;
(2) $M = \mathbb{R}_t \times]0, 1[_{\mathrm{x}}$: $J_+(x) \cap J_-(x')$ may not be compact;
(3) $M = \mathbb{S}^1_t \times \mathbb{R}_{\mathrm{x}}$: $J_\pm(x) = M$.



(1) $\mathbb{R}^{1,1} \backslash \{x_0\}$ (2) $\mathbb{R}_t \times]0, 1[_{\mathrm{x}}$ (3) $\mathbb{S}^1_t \times \mathbb{R}_{\mathrm{x}}$

Fig. 3

Later on we will need the following result, which is proved in [**BGP**, Lemma A.5.7].

LEMMA 5.4.3. *Let (M, g) be globally hyperbolic and $K_1, K_2 \Subset M$ be compact. Then $J_+(K_1) \cap J_-(K_2)$ is compact.*

The following theorem is also due to Bernal and Sanchez [**BS1, BS2**]. It extends an earlier result of Geroch [**Ge**].

THEOREM 5.4.4. *The following conditions are equivalent:*
(1) *(M, g) is globally hyperbolic.*
(2) *M admits a Cauchy surface S.*
(3) *There exists an isometric diffeomorphism:*

$$\chi : (M, g) \longrightarrow (\mathbb{R} \times \Sigma, -\beta(t, \mathrm{x})dt^2 + h_t(\mathrm{x})d\mathrm{x}^2),$$

where Σ is a smooth $(n-1)$-dimensional manifold, $\beta > 0$ is a smooth function on $\mathbb{R} \times \Sigma$, $t \mapsto h_t(\mathrm{x})d\mathrm{x}^2$ is a smooth family of Riemannian metrics on Σ, and $\{T\} \times \Sigma$ is a smooth space-like Cauchy surface in $\mathbb{R} \times \Sigma$ for each $T \in \mathbb{R}$.

5.4.1. Orthogonal decompositions of the metric. An isometry $\chi : M \to \mathbb{R} \times \Sigma$ such that $g = \chi^*(-\beta dt^2 + h_t d\mathrm{x}^2)$ as in Theorem 5.4.4 is called an *orthogonal decomposition*. Orthogonal decompositions are very useful to analyze Klein-Gordon equations on (M, g). The decomposition in Theorem 5.4.4 is related to the notion of *temporal functions*.

DEFINITION 5.4.5. *A smooth function $t : M \to \mathbb{R}$ is called a* temporal function *if its gradient $\nabla t = g^{-1}dt$ is everywhere time-like and past directed. It is called a* Cauchy temporal function *if, in addition, its level sets $t^{-1}(T)$ are Cauchy surfaces for all $T \in t(M)$.*

Clearly, if $\chi : M \to \mathbb{R} \times \Sigma$ is the diffeomorphism in Theorem 5.4.4 (3), then $t = \pi_{\mathbb{R}} \circ \chi$ is a Cauchy temporal function.

Now let t be a Cauchy temporal function. Without loss of generality we can assume that $t(M) = \mathbb{R}$ and set $\Sigma := t^{-1}(\{0\})$, which is a smooth, space-like Cauchy surface. We equip M with an auxiliary complete Riemannian metric $\hat{h}$ and set

$$v = \|\nabla t\|_{\hat{h}}^{-1} \nabla t,$$

which is a complete, time-like vector field. Since Σ is a Cauchy surface, its integral curve through $x \in M$ intersects Σ at a unique point $\psi(x) \in \Sigma$, and we set

$$\chi : M \ni x \longmapsto (t(x), \psi(x)) \in \mathbb{R} \times \Sigma,$$

which is a smooth diffeomorphism. If we set $\Sigma_s = t^{-1}(\{s\})$, then $T_x\Sigma_s$ is orthogonal to $\mathbb{R}v(x)$, hence is space-like by Lemma 5.2.3. The image of $T_x\Sigma_s$, resp. $\mathbb{R}v(x)$, under $D_x\chi$ is $\{0\} \times T_{\mathrm{y}}\Sigma$, resp. $\mathbb{R} \times \{0\}$. Therefore, the metric $(\chi^{-1})^* g$ is of the form $-\beta dt^2 + h_t$, with β and $t \mapsto h_t$ as in Theorem 5.4.4.

It is known, see [**BS4**, Theorem 1.2], that for any smooth, space-like Cauchy surface Σ, there exists a Cauchy temporal function $t : M \to \mathbb{R}$ such that $\Sigma = t^{-1}(\{0\})$.

Therefore, any smooth space-like Cauchy surface Σ can be chosen in Theorem 5.4.4 (3), and the isometry χ is completely determined by fixing Σ and a Cauchy temporal function t with $\Sigma = t^{-1}(\{0\})$.

5.4.2. Neighborhoods of a space-like Cauchy surface.

LEMMA 5.4.6. *Let $\Sigma \subset M$ be a smooth, space-like Cauchy surface. Then the open neighborhoods V of Σ such that $V \subset M$ is causally compatible form a basis of neighborhoods of Σ in M.*

Proof. We can assume that $M = \mathbb{R} \times \Sigma$ with metric $-\beta dt^2 + h_t d\mathrm{x}^2$ and identify Σ with $\{0\} \times \Sigma$. We can also assume that $\beta = 1$ by a conformal transformation. If U is a neighborhood of Σ, we can find a strictly positive function $r \in C^\infty(\Sigma)$ such that for $V := \{(t, \mathrm{x}) : |t| < r(\mathrm{x})\}$ one has

$$\begin{aligned} &\text{(i)} \quad V \subset U, \\ &\text{(ii)} \quad \tfrac{1}{4} h_0(\mathrm{x}) \leq h_t(\mathrm{x}) \leq 4 h_0(\mathrm{x}), \ \forall\, (t, \mathrm{x}) \in V, \\ &\text{(iii)} \quad \nabla r(\mathrm{x}) \cdot h_0(\mathrm{x}) \nabla r(\mathrm{x}) \leq \tfrac{1}{16}, \ \forall\, \mathrm{x} \in \Sigma. \end{aligned} \tag{5.16}$$

In fact, it suffices to fix an open covering $\{U_i\}_{i\in\mathbb{N}}$ of Σ and intervals $\{I_i\}_{i\in\mathbb{N}}$ such that $\bigcup_{i\in\mathbb{N}} I_i \times U_i \subset U$ and choose $r = \sum_{i\in\mathbb{N}} \epsilon_i \chi_i$, where $\{\chi_i\}_{i\in\mathbb{N}}$ is a partition of unity of Σ subordinate to $\{U_i\}_{i\in\mathbb{N}}$ and the ϵ_i are chosen small enough.

Let now $\gamma : [-1, 1] \ni s \mapsto x(s)$ be a future directed causal curve in (M, g) with $x(0), x(1) \in V$. Since Σ is a Cauchy surface, we can assume, modulo a reparametrization of γ, that $\pm t(s) \geq 0$ for $\pm s \in [0, 1]$. By (5.16) (ii), we have

$$t'(s) \geq \frac{1}{2} (\mathrm{x}'(s) \cdot h_0(\mathrm{x}(s)) \mathrm{x}'(s))^{\frac{1}{2}} \text{ for } s \in [-1, 1].$$

If $f(s) = t(s) - r(\mathrm{x}(s))$ for $s \in [0, 1]$, then we deduce from (5.16) (iii) and the Cauchy-Schwarz inequality that $f'(s) > 0$ as long as $s \in [0, 1]$ and $f(s) < 0$. Since $x(1) \in V$, we have $f(1) < 0$, hence $f(s) < 0$ for $s \in [0, 1]$, i.e. $x(s) \in V$ for $s \in [0, 1]$. For $s \in [-1, 0]$ we use the same argument for $f(s) = t(s) + r(\mathrm{x}(s))$. □

5.4.3. Gaussian normal coordinates. If $\Sigma \subset M$ is a smooth space-like Cauchy surface, there is another orthogonal decomposition of the metric using *Gaussian normal coordinates* to Σ. It does not depend on the choice of a Cauchy temporal function having Σ as one of its level sets, but Gaussian normal coordinates exist only in a neighborhood of Σ in M. Let $n \in T_\Sigma M$ be the future directed unit normal vector field to Σ, so that n_y is g-orthogonal to $T_y\Sigma$, future directed, and satisfies $n_y \cdot g(y) n_y = -1$. We denote by $\exp_x^g$ for $x \in M$ the exponential map at x for the metric g.

PROPOSITION 5.4.7. *Let $\Sigma \subset M$ be a smooth space-like Cauchy surface. Then*

(1) *there exist neighborhoods U of $\{0\} \times \Sigma$ in $\mathbb{R} \times \Sigma$ and V of Σ in M such that $V \subset M$ is causally compatible and*

$$\chi : U \ni (t, \mathrm{x}) \longmapsto \exp_{\mathrm{x}}^g(t n_{\mathrm{x}}) \in V \text{ is a diffeomorphism;}$$

(2) *one has $\chi^* g = -dt^2 + h_t(\mathrm{x}) d\mathrm{x}^2$, where h_t is a t-dependent Riemannian metric on Σ over U.*

Proof. The map χ is clearly a local diffeomorphism. The existence of U, V as in (1) is shown in [**O**, Proposition 26, Chap. 7] , and V can be chosen to be causally compatible in M by Lemma 5.4.6.

Let us explain the proof of (2), following [**W1**, Section 3.3]. Using local coordinates x^i, $1 \leq i \leq n-1$ on Σ near a point $y \in \Sigma$ we obtain by means of χ local coordinates t, x^i near a point $x \in V$. Let $T = \partial_t, X_i = \partial_{x^i}$ be the associated coordinate vector fields. Recall that if ∇ is the Levi-Civita connection, then

$$T^b \nabla_b T^a = 0, \tag{5.17}$$

$$T^b \nabla_b X_i^a - X_i^b \nabla_b T^a = [T, X_i]^a = 0. \tag{5.18}$$

(5.17) is the geodesic equation, and the Lie bracket $[T, X_i]$ vanishes since T, X_i are coordinate vector fields. Denoting by $X = X^a$ one of the vector fields X_i, we compute:

$$T^b \nabla_b (T_a X^a) = X^a T^b \nabla_b T_a + T_a T^b \nabla_b X^a = T_a T^b \nabla_b X^a,$$

using (5.17) and $\nabla_a g_{bc} = 0$. Next,

$$T_a T^b \nabla_b X^a = X^b T_a \nabla_b T^a = \frac{1}{2} X^b \nabla_b (T^a T_a),$$

by (5.18) and the Leibniz rule for ∇. Finally, since $T^a T_a = -1$ on Σ and $T^b \nabla_b (T^a T_a) = 0$, we have $T^a T_a = -1$ everywhere, which implies that $T^b \nabla_b (T_a X^a) = 0$. Since $T_a X^a = 0$ on Σ, we obtain $T_a X^a = 0$, $T^a T_a = -1$ everywhere. This implies (2). □

5.4.4. Spaces of distributions on globally hyperbolic spacetimes. We now recall some useful spaces of distributions on M, characterized by their support properties. We refer the reader to [**S1**, Section 4] for a complete discussion.

Definition 5.4.8. *A distribution $u \in \mathcal{D}'(M)$ is space, (time), future/past compact if its support is space, (time), future/past compact. The spaces of such distributions are denoted by $\mathcal{D}'_{\mathrm{sc}}(M)$, $\mathcal{D}'_{\mathrm{tc}}(M)$, $\mathcal{D}'_{\mathrm{sc},\pm}(M)$, $\mathcal{D}'_{\mathrm{tc},\pm}(M)$. Similarly, one defines the space, of smooth functions $C^\infty_{\mathrm{sc}}(M)$, $C^\infty_{\mathrm{tc}}(M)$, $C^\infty_{\mathrm{sc},\pm}(M)$, $C^\infty_{\mathrm{tc},\pm}(M)$.*

The most useful space is $C^\infty_{\mathrm{sc}}(M)$; the other spaces appear naturally when discussing properties of the *retarded/advanced inverses* for Klein-Gordon operators, see Section 5.5 below.

It is proved in [**S1**, Theorem 3.1] that a closed set $A \subset M$ is future/past time compact iff there exists a Cauchy surface Σ in M such that $A \subset J_\pm(\Sigma)$.

Now let us describe the topologies of these spaces. If $B \subset M$ is closed, we denote by $C^\infty(B)$, resp. $\mathcal{D}'(B)$, the smooth functions, resp. distributions with support in B, equipped with the $C^\infty(M)$, resp. $\mathcal{D}'(M)$ topology. The topologies of the above spaces are defined as the following inductive limits:

(5.19)

(i) $C^\infty_{\mathrm{sc}}(M) = \bigcup_{K \Subset M} C^\infty(J(K))$, $\mathcal{D}'_{\mathrm{sc}}(M) = \bigcup_{K \Subset M} \mathcal{D}'(J(K))$,

(ii) $C^\infty_{\mathrm{sc},+}(M) = \bigcup_{K \Subset M} C^\infty(J_-(K))$, $\mathcal{D}'_{\mathrm{sc},+}(M) = \bigcup_{K \Subset M} \mathcal{D}'(J_-(K))$,

(iii) $C^\infty_{\mathrm{sc},-}(M) = \bigcup_{K \Subset M} C^\infty(J_+(K))$, $\mathcal{D}'_{\mathrm{sc},-}(M) = \bigcup_{K \Subset M} \mathcal{D}'(J_+(K))$,

(iv) $C^\infty_{\mathrm{tc},+}(M) = \bigcup_{\Sigma \subset M} C^\infty(J_-(\Sigma))$, $\mathcal{D}'_{\mathrm{tc},+}(M) = \bigcup_{\Sigma \subset M} \mathcal{D}'(J_-(\Sigma))$,

(v) $C^\infty_{\mathrm{tc},-}(M) = \bigcup_{\Sigma \subset M} C^\infty(J_+(\Sigma))$, $\mathcal{D}'_{\mathrm{tc},-}(M) = \bigcup_{\Sigma \subset M} \mathcal{D}'(J_+(\Sigma))$,

(vi) $C^\infty_{\mathrm{tc}}(M) = \bigcup_{\Sigma_1,\Sigma_2 \subset M} C^\infty(J_+(\Sigma_1) \cap J_-(\Sigma_2))$,

(vii) $\mathcal{D}'_{\mathrm{tc}}(M) = \bigcup_{\Sigma_1,\Sigma_2 \subset M} \mathcal{D}'(J_+(\Sigma_1) \cap J_-(\Sigma_2))$.

In (i), (ii), and (iii) the set of compact subsets $K \Subset M$ is equipped with the order relation $K_1 \leq K_2$ if $K_1 \subset K_2$; in (iv), resp. (v) the set of Cauchy surfaces $\Sigma \subset M$ is equipped with the order relation $\Sigma \leq \Sigma'$ if $J_-(\Sigma) \subset J_-(\Sigma')$, resp. $J_+(\Sigma) \subset J_+(\Sigma')$; and finally, in (vi) and (vii) the set of pairs of Cauchy surfaces (Σ_1, Σ_2) is equipped with the order relation $(\Sigma_1, \Sigma_2) \leq (\Sigma'_1, \Sigma'_2)$ if $J_+(\Sigma_1) \cap J_-(\Sigma_2) \subset J_+(\Sigma'_1) \cap J_-(\Sigma'_2)$.

The various duality relations between these spaces are as follows, see [**S1**, Theorem 4.3].

Proposition 5.4.9. *One has*

$$\mathcal{D}'_{\mathrm{sc}}(M) = C^\infty_{\mathrm{tc}}(M)', \quad \mathcal{D}'_{\mathrm{tc}}(M) = C^\infty_{\mathrm{sc}}(M)',$$
$$\mathcal{D}'_{\mathrm{sc},\pm}(M) = C^\infty_{\mathrm{tc},\mp}(M)', \quad \mathcal{D}'_{\mathrm{tc},\pm}(M) = C^\infty_{\mathrm{sc},\mp}(M)',$$

and all the spaces above are reflexive.

5.5. Klein-Gordon equations on Lorentzian manifolds

5.5.1. Klein-Gordon operator. Let us fix a smooth real 1-form $A = A_\mu(x)dx^\mu$ on M and a real function $V \in C^\infty(M;\mathbb{R})$. A *Klein-Gordon operator* on (M,g) is a differential operator

$$P = -(\nabla^\mu - \mathrm{i}qA^\mu(x))(\nabla_\mu - \mathrm{i}qA_\mu(x)) + V(x), \tag{5.20}$$

where $\nabla^\mu = |g|^{-\frac{1}{2}}(x)\nabla_\nu|g|^{\frac{1}{2}}(x)g^{\mu\nu}(x)$, $A^\mu(x) = g^{\mu\nu}(x)A_\nu(x)$, and $q \in \mathbb{R}$.

The quantization of the Klein-Gordon equation $P\phi = 0$ for $\phi \in C^\infty(M;\mathbb{C})$ describes a charged bosonic field of charge q in the external electro-magnetic potential $A_\mu(x)dx^\mu$. If $A_\mu(x)dx^\mu = 0$, then $P = -\Box_g + V(x)$, where $\Box_g = \nabla^\mu\nabla_\mu$ is the d'Alembertian. A typical example of V is $V = \xi\mathrm{Scal}_g + m^2$, where Scal_g is the scalar curvature on (M,g), which for $\xi = \frac{n-2}{4(n-1)}, m = 0$ yields the *conformal wave operator*.

Recall that we defined the scalar product

$$(u|v)_M = \int_M \overline{u}v dVol_g,$$

on $C_0^\infty(M)$. Clearly, P is formally selfadjoint with respect to $(\cdot|\cdot)_M$.

Actually, every differential operator of the form

$$P = -\Box_g + R(x,\partial_x),$$

where $R(x,\partial_x)$ is a first-order differential operator on M such that P is formally selfadjoint with respect to $(\cdot|\cdot)_M$, is of the form (5.20).

We are interested in the Klein-Gordon equation

$$P\phi = 0,$$

and we will always consider its *complex* solutions in $\mathcal{D}'(M)$ or $C^\infty(M)$.

5.5.2. Conserved currents. Let us set

$$\nabla_a^A := \nabla_a - \mathrm{i}qA_a, \quad \nabla^{aA} := \nabla^a - \mathrm{i}qA^a$$

and introduce on M the 1-form

$$J_a(u_1,u_2) := \nabla_a^A\overline{u}_1u_2 - \overline{u}_1\nabla_a^Au_2,\ u_1,u_2 \in C^\infty(M). \tag{5.21}$$

We have

$$\nabla^{aA}J_a(u_1,u_2) = -\overline{u}_1Pu_2 + \overline{Pu_1}u_2. \tag{5.22}$$

It follows that if $u_i \in C^\infty(M)$ with $Pu_i \in C_0^\infty(M)$ and $U \subset M$ is an open set with ∂U a finite union of non-characteristic hypersurfaces, we obtain from Subsection 5.2.4 the *Green formula*

$$\int_U \big(\overline{u}_1Pu_2 - \overline{Pu_1}u_2\big)dVol_g = \int_{\partial U}\big(n^a\nabla_a^A\overline{u}_1u_2 - \overline{u}_1n^a\nabla_a^Au_2\big)dVol_h, \tag{5.23}$$

where h is the induced metric on ∂U.

To have a satisfactory global theory of Klein-Gordon equations on M, we need to make some assumptions on its causal structure. It turns out that if (M,g) is globally hyperbolic the theory is particularly nice and complete.

5.5.3. Advanced and retarded inverses. The following extension of Theorem 2.2.2 is originally due to Leray [**Le**]. A proof can be found in [**BGP**, Theorem 3.3.1].

THEOREM 5.5.1. *Let (M, g) be globally hyperbolic and let P be a Klein-Gordon operator on M. Then for $v \in \mathcal{E}'(M)$ there exist unique solutions $u_{\mathrm{ret/adv}} \in \mathcal{D}'_{\mathrm{sc},\pm}(M)$ of the equation*

$$Pu_{\mathrm{ret/adv}} = v.$$

One has $u_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}} v$, where

(5.24)

(i) $G_{\mathrm{ret/adv}} : \mathcal{E}'(M) \to \mathcal{D}'(M)$, $G_{\mathrm{ret/adv}} : C_0^\infty(M) \to C^\infty(M)$ *continuously*;

(ii) $P \circ G_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}} \circ P = \mathbb{1}$;

(iii) $\operatorname{supp} G_{\mathrm{ret/adv}} v \subset J_\pm(\operatorname{supp} v)$.

Using the continuity and support properties of $G_{\mathrm{ret/adv}}$ and the topologies of the spaces introduced in Definition 5.4.8, one easily obtains the following corollary.

COROLLARY 5.5.2. *The maps $G_{\mathrm{ret/adv}}$ extend continuously as follows*

$$\begin{aligned} G_{\mathrm{ret/adv}} : \quad & C^\infty_{\mathrm{sc},\pm}(M) \longrightarrow C^\infty_{\mathrm{sc},\pm}(M), \quad \mathcal{D}'_{\mathrm{sc},\pm}(M) \longrightarrow \mathcal{D}'_{\mathrm{sc},\pm}(M), \\ G_{\mathrm{ret/adv}} : \quad & C^\infty_{\mathrm{tc},\pm}(M) \longrightarrow C^\infty_{\mathrm{tc},\pm}(M), \quad \mathcal{D}'_{\mathrm{tc},\pm}(M) \longrightarrow \mathcal{D}'_{\mathrm{tc},\pm}(M) \end{aligned}$$

The operator

$$G = G_{\mathrm{ret}} - G_{\mathrm{adv}} \tag{5.25}$$

is called in physics the *Pauli-Jordan function* or *causal propagator*. Using that $P = P^*$ and the uniqueness of $G_{\mathrm{ret/adv}}$, we obtain that $G_{\mathrm{ret/adv}} = G^*_{\mathrm{adv/ret}}$ on $C_0^\infty(M)$, hence

$$G = -G^*, \quad \operatorname{supp} Gv \subset J(\operatorname{supp} v). \tag{5.26}$$

5.5.4. The Cauchy problem. We now discuss the Cauchy problem for P. Let Σ be a smooth, space-like Cauchy surface in M, n the future unit normal to Σ, see Subsection 5.4.3, and $\partial_n^A = n^a \nabla_a^A$. As in Section 2.4, we define the Cauchy data map ϱ_Σ by:

$$\varrho_\Sigma \phi := \begin{pmatrix} \phi\restriction_\Sigma \\ \mathrm{i}^{-1} \partial_n^A \phi\restriction_\Sigma \end{pmatrix}, \quad \phi \in C^\infty(M). \tag{5.27}$$

The proof of the following result can be found in [**BGP**, Theorem 3.2.11].

THEOREM 5.5.3. *The Cauchy problem*

$$\begin{cases} P\phi = 0, \\ \varrho_\Sigma \phi = f, \end{cases} \tag{5.28}$$

has a unique solution $\phi = U_\Sigma f \in C^\infty(M)$ for each $f = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} \in C_0^\infty(\Sigma; \mathbb{C}^2)$. Moreover the map $U_\Sigma : C_0^\infty(\Sigma; \mathbb{C}^2) \to C^\infty(M)$ is continuous and

$$\operatorname{supp} U_\Sigma f \subset J(\operatorname{supp} f_0 \cap \operatorname{supp} f_1).$$

Let us recall a well-known relation between the Cauchy evolution operator U_Σ and G. We first introduce some notation. Since $\varrho_\Sigma : C_0^\infty(M) \to C_0^\infty(\Sigma; \mathbb{C}^2)$ we obtain by duality the map

$$\varrho_\Sigma^* : \mathcal{D}'(\Sigma; \mathbb{C}^2) \longrightarrow \mathcal{D}'(M), \tag{5.29}$$

where in (5.29) we identify the space $C_0^\infty(M)'$ (resp. $C_0^\infty(\Sigma)'$), of distribution densities on M (resp. on Σ), with $\mathcal{D}'(M)$ (resp. $\mathcal{D}'(\Sigma)$) using the density $dVol_g$ (resp. $dVol_h$). A concrete expression of ϱ_Σ^* is

$$\varrho_\Sigma^* f = f_0 \otimes \delta_\Sigma + \mathrm{i}^{-1} f_1 \otimes n\cdot\nabla\delta_\Sigma, \tag{5.30}$$

where the distribution δ_Σ is defined by

$$\langle \delta_\Sigma dVol_g, u\rangle = \int_\Sigma u\, dVol_h, \quad u \in C_0^\infty(M).$$

We also set

$$q_\Sigma := \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \in L(C_0^\infty(\Sigma;\mathbb{C}^2)). \tag{5.31}$$

Proposition 5.5.4. *Set $G_\Sigma = \mathrm{i}^{-1} q_\Sigma$. Then*

$$U_\Sigma = (\varrho_\Sigma G)^* G_\Sigma, \quad \text{on } C_0^\infty(\Sigma;\mathbb{C}^2).$$

Proof. We apply Green's formula (5.23) to $u_2 = u = U_\Sigma f$, $u_1 = G_{\mathrm{adv/ret}} v$, $v \in C_0^\infty(M)$ and $U = J_\pm(\Sigma)$. This yields

$$\int_{J_+(\Sigma)} \overline{v} u\, dVol_g = \int_\Sigma \big(- \overline{G_{\mathrm{adv}} v} n^a \nabla_a^A u + \overline{n^a \nabla_a^A G_{\mathrm{adv}} v} u\big) dVol_h,$$
$$\int_{J_-(\Sigma)} \overline{v} u\, dVol_g = \int_\Sigma \big(\overline{G_{\mathrm{ret}} v} n^a \nabla_a^A u - \overline{G_{\mathrm{ret}} v} n^a \nabla_a^A u\big) dVol_h.$$

Adding the two equations above, we get, since $J(\Sigma) = M$,

$$\int_M \overline{v} u dVol_g = -\int_\Sigma n^a J_a(Gv, u) dVol_h.$$

By the definition of ϱ_Σ^* and the fact that $G = -G^*$ we obtain the proposition. □

From Proposition 5.5.4 and Corrollary 5.5.2 we obtain the following continuous extensions of U_Σ:

$$U_\Sigma : \mathcal{E}'(\Sigma;\mathbb{C}^2) \longrightarrow \mathcal{D}'_{\mathrm{sc}}(M), \quad \mathcal{D}'(\Sigma;\mathbb{C}^2) \longrightarrow \mathcal{D}'(M). \tag{5.32}$$

5.6. Symplectic spaces

5.6.1. Symplectic space of Cauchy data. We equip $C_0^\infty(\Sigma;\mathbb{C}^2)$ with the Hermitian form

$$\overline{g}\cdot q_\Sigma f := \int_\Sigma \big(\overline{g}_1 f_0 + \overline{g}_0 f_1\big) dVol_h. \tag{5.33}$$

Abusing the notation, we have

$$\overline{g}\cdot q_\Sigma f = (g|q_\Sigma f)_\Sigma,$$

for

$$(g|f)_\Sigma = \int_\Sigma \big(\overline{g}_0 f_0 + \overline{g}_1 f_1\big) dVol_h, \tag{5.34}$$

and the operator q_Σ is defined in (5.31). Clearly, $(C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma)$ is a Hermitian space, see Subsection 4.2.4.

5.6.2. Symplectic space of solutions. Let us denote by $\mathrm{Sol}_{\mathrm{sc}}(P)$ the space of smooth complex space-compact solutions of the Klein-Gordon equation $P\phi = 0$.

PROPOSITION 5.6.1. (1) *The Hermitian form q on $\mathrm{Sol}_{\mathrm{sc}}(P)$ defined by:*

$$\overline{\phi}_1 \cdot q\phi_2 = \mathrm{i}\int_\Sigma n^a J_a^A(\phi_1,\phi_2) dVol_h \tag{5.35}$$

is independent on the choice of the space-like Cauchy surface Σ and $(\mathrm{Sol}_{\mathrm{sc}}(P), q)$ is a Hermitian space.

(2) *If Σ is a space-like Cauchy surface, the map*

$$\varrho_\Sigma : (C_0^\infty(\Sigma;\mathbb{C}^2, q_\Sigma) \longrightarrow (\mathrm{Sol}_{\mathrm{sc}}(P), q)$$

is unitary with inverse U_Σ.

Proof. If $\phi_1, \phi_2 \in \mathrm{Sol}_{\mathrm{sc}}(P)$, then by (5.22) we have $\nabla_a^A J^a(\phi_1,\phi_2) = 0$. If Σ, Σ' are two space-like Cauchy surfaces with $\Sigma' \subset J_+(\Sigma)$, we apply the Gauss formula to $U = \mathrm{Int}(J_+(\Sigma) \cap J_-(\Sigma'))$ and obtain that

$$\int_\Sigma n^a J_a^A(\phi_1,\phi_2) dVol_h = \int_{\Sigma'} n^a J_a^A(\phi_1,\phi_2) dVol_h.$$

In the general case we pick another Cauchy surface $\Sigma'' \subset J_+(\Sigma) \cap J_+(\Sigma')$ and apply the same argument to obtain (1). Statement (2) follows immediately. □

5.6.3. Pre-symplectic space of test functions.

THEOREM 5.6.2. (1) *The sequence*

$$0 \longrightarrow C_0^\infty(M) \xrightarrow{P} C_0^\infty(M) \xrightarrow{G} C_{\mathrm{sc}}^\infty(M) \xrightarrow{P} C_{\mathrm{sc}}^\infty(M) \longrightarrow 0$$

is an exact complex.

(2) *Let Σ be a space-like Cauchy surface. Then one has*

$$(\varrho_\Sigma G)^* G_\Sigma(\varrho_\Sigma G) = G \text{ on } C_0^\infty(M).$$

(3) *The map*

$$G : (\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\mathrm{i}G\,\cdot)_M) \longrightarrow (\mathrm{Sol}_{\mathrm{sc}}(P), q)$$

is unitary.

Proof. (1) The above sequence is clearly a complex since $G \circ P = 0$ and $P \circ G = 0$ on $C_0^\infty(M)$. Let us check that it is exact.

Let $u \in C_0^\infty(M)$ with $Pu = 0$. Since $u \in C_{\mathrm{sc}}^\infty(M)$ we have $u = G_{\mathrm{ret}} 0 = 0$ by Theorem 5.5.1, which proves exactness at the first $C_0^\infty(M)$.

Let $u \in C_0^\infty(M)$ with $Gu = 0$. We have $v := G_{\mathrm{ret}} u = G_{\mathrm{adv}} u \in C_0^\infty(M)$ since $\mathrm{supp}\, v \subset J_+(\mathrm{supp}\, u) \cap J_-(\mathrm{supp}\, u)$ is compact by Lemma 5.4.3. Then $u = Pv$, and so $u \in PC_0^\infty(M)$, which proves exactness at the second $C_0^\infty(M)$.

Let $\phi \in C_{\mathrm{sc}}^\infty(M)$ with $P\phi = 0$, i.e. $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$. We can find cutoff functions $\chi_\pm \in C_{\mathrm{sc},\pm}^\infty(M)$ such that $\chi_+ + \chi_- = 1$ on $\mathrm{supp}\,\phi$, see Fig. 4 below. We have $\mathrm{supp}\,\phi \subset J(K)$ and $\mathrm{supp}\,\chi_\pm \subset J_\pm(K_\pm)$ for $K, K_\pm$ compact. Since $\nabla\chi_+ = -\nabla\chi_-$ on $\mathrm{supp}\,\phi$ we have $\mathrm{supp}\,\phi \cap \mathrm{supp}\,\nabla\chi_\pm \subset J(K) \cap J_+(K_+) \cap J_-(K_-)$ which is compact by Lemma 5.4.3. We set $\phi_\pm = \chi_\pm\phi$ and $v = P\phi_+ = -P\phi_-$, which belongs to $C_0^\infty(M)$, by the compactness of $\mathrm{supp}\,\phi \cap \mathrm{supp}\,\nabla\chi_\pm$. Since $\phi_\pm \in C_{\mathrm{sc},\pm}^\infty(M)$ we have $\phi_\pm = \pm G_{\mathrm{ret/adv}} v$ hence $\phi = Gv$, which proves exactness at the first $C_{\mathrm{sc}}^\infty(M)$.

Let $v \in C_{\mathrm{sc}}^\infty(M)$ and $\chi_\pm \in C_{\mathrm{sc},\pm}^\infty(M)$ such that $\chi_+ + \chi_- = 1$ on $\mathrm{supp}\, v$. From Theorem 5.5.1 (iii) we see that $G_{\mathrm{ret/adv}}$ can be extended as a map from $C_{\mathrm{sc},\mp}^\infty(M)$ to $C_{\mathrm{sc},\pm}^\infty(M)$. We set then $u = G_{\mathrm{ret}}\chi_- v + G_{\mathrm{adv}}\chi_+ v$ and $Pu = v$, $u \in C_{\mathrm{sc}}^\infty(M)$ which proves exactness at the second $C_{\mathrm{sc}}^\infty(M)$.

(2) From $U_\Sigma \varrho_\Sigma = \mathbb{1}$ on $\mathrm{Sol}_{\mathrm{sc}}(P)$, $U_\Sigma = (\varrho_\Sigma G)^* G_\Sigma$ on $C_0^\infty(\Sigma;\mathbb{C}^2)$ and $\mathrm{Sol}_{\mathrm{sc}}(P) = GC_0^\infty(M)$ we obtain (2).

(3) The map G and the Hermitian form $(\cdot\,|\mathrm{i}G\,\cdot)_M$ are well defined on $\frac{C_0^\infty(M)}{PC_0^\infty(M)}$ since $G\circ P = P\circ G = 0$. By (1), the map $G : \frac{C_0^\infty(M)}{PC_0^\infty(M)} \to \mathrm{Sol}_{\mathrm{sc}}(P)$ is bijective, and by (2) and the definition of q in (5.35), it is unitary. □

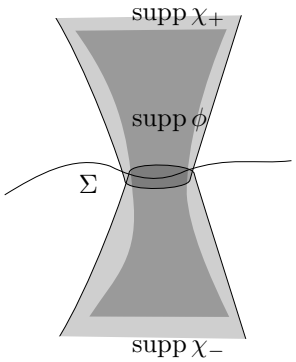


Fig. 4

Let us summarize the above discussion.

THEOREM 5.6.3. *The maps*

$$\Big(\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\mathrm{i}G\,\cdot)_M\Big) \xrightarrow{G} (\mathrm{Sol}_{\mathrm{sc}}(P), q) \xrightarrow{\rho_\Sigma} (C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma)$$

are isomorphisms of Hermitian spaces.

As in the Minkowski case, the first and last Hermitian spaces are the most useful.

5.6.4. Time-slice property. We end this subsection with a remark which is related to the *time-slice axiom* see e.g. [**BGP**, Theorem 4.5.1].

PROPOSITION 5.6.4. *Let Σ a space-like Cauchy surface and $V \subset M$ a neighborhood of Σ such that $V \subset M$ is causally compatible. Then the maps*

$$\Big(\frac{C_0^\infty(V)}{PC_0^\infty(V)}, (\cdot\,|\mathrm{i}G\,\cdot)_M\Big) \xrightarrow{G} (\mathrm{Sol}_{\mathrm{sc}}(P), q) \xrightarrow{\rho_\Sigma} (C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma)$$

are isomorphisms of Hermitian spaces.

Proof. The space (V, g) is globally hyperbolic. Let $P|_V$ be the restriction of P to V. Since $V \subset M$ is causally compatible, the causal propagator for $P|_V$ equals $G|_V$. If $[u] \in \frac{C_0^\infty(V)}{PC_0^\infty(V)}$, then $G|_V u = (Gu)|_V$. Applying this remark and Theorem 5.6.3 for V we obtain the proposition. □

CHAPTER 6

Quasi-free states on curved spacetimes

We saw in Chapter 5 that to a Klein-Gordon operator P on a globally hyperbolic spacetime (M,g) one can associate the Hermitian space $(\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\mathrm{i}G\,\cdot)_M)$. Following Chapter 4, one can then consider the associated CCR $*$-algebra and quasi-free states on it.

The complex covariances of a quasi-free state induce sesquilinear forms on $C_0^\infty(M)$ and it is natural to assume their continuity for the topology of $C_0^\infty(M)$, which allows to introduce their distributional kernels.

By Proposition 5.6.4 one can equivalently use the Hermitian space $(C_0^\infty(\Sigma,\mathbb{C}^2), q_\Sigma)$ if Σ is a space-like Cauchy surface. The associated covariances are called *Cauchy surface covariances* and are very useful for the concrete construction of states.

6.1. Quasi-free states on curved spacetimes

Definition 6.1.1. *We denote by* $\mathrm{CCR}(P)$ *the* $*$*-algebra* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},q)$*, see Subsection 4.5.3, for*

$$(\mathcal{Y},q)=(\frac{C_0^\infty(M)}{PC_0^\infty(M)},(\cdot\,|\mathrm{i}G\,\cdot)_M).$$

6.1.1. Space-time covariances. We will identify distribution densities on M, resp. $M\times M$ with distributions using the density $dVol_g$, resp. $dVol_g\times dVol_g$.

Let ω be a gauge invariant quasi-free state on $\mathrm{CCR}(P)$. Its complex covariances are sesquilinear forms on $\frac{C_0^\infty(M)}{PC_0^\infty(M)}$, or equivalently sesquilinear forms $\Lambda^\pm$ on $C_0^\infty(M)$ such that

$$\overline{u}\cdot\Lambda^\pm Pv=\overline{Pu}\cdot\Lambda^\pm v=0,\quad u,v\in C_0^\infty(M),$$

or in more compact notation $\Lambda^\pm\circ P=P^*\circ\Lambda^\pm$, where P^* is the formal adjoint of P defined in Subsection 4.1.4.

It is natural to require that $\Lambda^\pm: C_0^\infty(M)\to\mathcal{D}'(M)$ are continuous, which we will always assume in the sequel. By the Schwartz kernel theorem, $\Lambda^\pm$ have distributional kernels, still denoted by $\Lambda^\pm\in\mathcal{D}'(M\times M)$, defined by

$$\overline{u}\cdot\Lambda^\pm v=:(\Lambda^\pm|\overline{u}\otimes v)_{M\times M},\quad u,v\in C_0^\infty(M). \tag{6.1}$$

Definition 6.1.2. *The maps* $\Lambda^\pm: C_0^\infty(M)\to\mathcal{D}'(M)$ *are called the* spacetime covariances *of* ω*.*

By Proposition 4.7.6 we have:

Proposition 6.1.3. *Two maps* $\Lambda^\pm: C_0^\infty(M)\to\mathcal{D}'(M)$ *are the spacetime covariances of a gauge invariant quasi-free state* ω *iff*

(i) $\Lambda^\pm: C_0^\infty(M)\to\mathcal{D}'(M)$ *are linear and continuous,*

(ii) $(u|\Lambda^\pm u)_M\geq 0,\ u\in C_0^\infty(M)$,

(iii) $\Lambda^+-\Lambda^-=\mathrm{i}G$,

(iv) $P\circ\Lambda^\pm=\Lambda^\pm\circ P=0$.

6.1.2. Cauchy surface covariances. Let $\Sigma \subset M$ a space-like Cauchy surface. We again identify distributions on Σ with distribution densities using the volume form $dVol_h$, where h is the induced Riemannian metric on Σ.

By Theorem 5.6.3, we can use equivalently the symplectic space $(C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma)$ to describe CCR(P). Therefore a quasi-free state ω as above can equivalently be defined by a pair $\lambda_\Sigma^\pm$ of sesquilinear forms on $C_0^\infty(\Sigma;\mathbb{C}^2)$, or equivalently linear maps $\lambda_\Sigma^\pm : C_0^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$. We will see later that $\Lambda^\pm : C_0^\infty(M) \to \mathcal{D}'(M)$ is linear and continuous iff $\lambda^\pm : C_0^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$ is linear and continuous.

Definition 6.1.4. *The maps $\lambda_\Sigma^\pm$ are called the* Cauchy surface covariances *of the state ω.*

We recall that the scalar product $(\cdot|\cdot)_\Sigma$ on $C_0^\infty(\Sigma;\mathbb{C}^2)$ was defined in (5.34).

Proposition 6.1.5. *Two maps $\lambda_\Sigma^\pm : C_0^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$ are the Cauchy surface covariances of a gauge invariant quasi-free state ω iff*

(i) $\lambda_\Sigma^\pm : C_0^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$ *are linear and continuous,*

(ii) $(f|\lambda_\Sigma^\pm f)_\Sigma \geq 0,\ f \in C_0^\infty(\Sigma;\mathbb{C}^2)$,

(iii) $\lambda_\Sigma^+ - \lambda_\Sigma^- = q_\Sigma$.

We recall that q_Σ is defined in (5.31) and that $G_\Sigma = \mathrm{i}^{-1} q_\Sigma$. Let us now look at the relationship between $\Lambda^\pm$ and $\lambda_\Sigma^\pm$.

Proposition 6.1.6. (1) *Let $\lambda_\Sigma^\pm$ be Cauchy surface covariances of a quasi-free state ω. Then*

$$\Lambda^\pm := (\varrho_\Sigma G)^* \lambda_\Sigma^\pm (\varrho_\Sigma G)$$

are the spacetime covariances of ω.

(2) *let $\Lambda^\pm$ be the spacetime covariances of a quasi-free state ω. Then*

$$\lambda_\Sigma^\pm := (\varrho_\Sigma^* G_\Sigma)^* \Lambda^\pm (\varrho_\Sigma^* G_\Sigma).$$

are the Cauchy surface covariances of ω.

Proof. (1) Since $\varrho_\Sigma^* \lambda_\Sigma^\pm \varrho_\Sigma G : C_0^\infty(M) \to \mathcal{D}'_{\mathrm{tc}}(M)$ and $\lambda_\Sigma^\pm : C^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$ are continuous, we see that $\Lambda^\pm : C_0^\infty(M) \to \mathcal{D}'(M)$ is continuous, by Corollary 5.5.2. The rest of the conditions in Proposition 6.1.3 follow from the equalities $P \circ G = G \circ P = 0$ and the fact that

$$\varrho_\Sigma G : \Big(\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\,\mathrm{i}G\,\cdot)_M\Big) \longrightarrow (C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma)$$

is unitary.

(2) The fact that $\lambda_\Sigma^\pm : C_0^\infty(\Sigma;\mathbb{C}^2) \to \mathcal{D}'(\Sigma;\mathbb{C}^2)$ is continuous uses properties of the *wavefront set* of $\Lambda^\pm$ deduced from the equalities $P \circ \Lambda^\pm = \Lambda^\pm \circ P = 0$ and will be explained later on in Chapter 7, see Subsection 7.2.9.

Item (ii) in Proposition 6.1.5 follows from item (ii) in Proposition 6.1.3. To check item (iii) in Proposition 6.1.5, we write

$$\lambda_\Sigma^+ - \lambda_\Sigma^- = (\varrho_\Sigma^* G_\Sigma)^* \mathrm{i} G (\varrho_\Sigma^* G_\Sigma) = -G_\Sigma \varrho_\Sigma \mathrm{i} G \varrho_\Sigma^* G_\Sigma = q_\Sigma,$$

since $\varrho_\Sigma(\varrho_\Sigma G)^* G_\Sigma = \mathbb{1}$, by Proposition 5.5.4. Therefore $\lambda_\Sigma^\pm$ are the Cauchy surface covariances of a quasi-free state ω_1. To check that $\omega_1 = \omega$, we use (1) and the fact that $\varrho_\Sigma(\varrho_\Sigma G)^* G_\Sigma = \mathbb{1}$ to conclude that $\Lambda^\pm$ are the spacetime covariances of ω_1, and hence $\omega_1 = \omega$. □

6.1.3. The case of real fields. For comparison with the literature, let us briefly explain the framework for *real* Klein-Gordon fields. Let P be a *real* Klein-Gordon operator, i.e. such that $\overline{Pu} = P\overline{u}$. Clearly, $G_{\mathrm{ret/adv}}$ and hence G are also real operators.

Consider the real symplectic space

$$(\mathcal{X}, \sigma) := (\frac{C_0^\infty(M;\mathbb{R})}{PC_0^\infty(M;\mathbb{R})}, (\cdot|G\cdot)_M),$$

and denote by $\mathrm{CCR}_{\mathbb{R}}(P)$ the $*$-algebra $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$. The real covariance of a quasi-free state ω is a (continuous) bilinear form H on $C_0^\infty(M;\mathbb{R})$, i.e. a continuous map $H : C_0^\infty(M;\mathbb{R}) \to \mathcal{D}'(M;\mathbb{R})$. It satisfies $H \circ P = P \circ H = 0$. The *two-point function* ω_2 of ω, defined by

$$\int_{M\times M} \omega_2(x,x')u(x)v(x')dVol_g \times dVol_g := \omega(\phi(u)\phi(v))$$

is equal by (4.15) to

$$\omega_2 = H + \frac{\mathrm{i}}{2}G,$$

and we denote by

$$\omega_{2\mathbb{C}} = H_{\mathbb{C}} + \frac{\mathrm{i}}{2}G_{\mathbb{C}} : C_0^\infty(M) \longrightarrow \mathcal{D}'(M)$$

its sesquilinear extension.

Let us formulate the version of Proposition 6.1.3 in the real case, which follows from Proposition 4.7.1.

Proposition 6.1.7. *A map $\omega_2 : C_0^\infty(M;\mathbb{R}) \to \mathcal{D}'(M;\mathbb{R})$ is the two-point function of a quasi-free state for the real Klein-Gordon operator P iff*

(i) $\omega_{2\mathbb{C}} : C_0^\infty(M) \to \mathcal{D}'(M)$ *is continuous,*

(ii) $(u|\omega_{2\mathbb{C}}u)_M \geq 0, \quad u \in C_0^\infty(M),$

(iii) $\omega_{2\mathbb{C}} - {}^t\omega_{2\mathbb{C}} = \mathrm{i}G_{\mathbb{C}}.$

6.2. Consequences of unique continuation

Next let us examine some consequences on $\mathrm{CCR}(P)$ of *unique continuation* results for the Klein-Gordon operator P. We first introduce some terminology taken from [**KW**, Section 2].

Definition 6.2.1. *Let $O \subset M$ be an open set. The* domain of determinacy *$\mathscr{D}(O)$ is the largest open set $U \subset M$ such that $P\phi = 0$, $\phi|_O = 0$ implies $\phi|_U = 0$ for all $\phi \in \mathcal{D}'(M)$.*

From the existence and uniqueness for the Cauchy problem, see Theorem 5.5.3, one sees that if Σ is a Cauchy surface in M, the interior of the *domain of dependence* $D(\Sigma \cap O)$, defined as the set $\{x \in M : J(x) \cap \Sigma \subset O\}$, is included in $\mathscr{D}(O)$. Also, if $O^\perp := \{x \in M : x \cap J(O) = \emptyset\}$ is the *causal complement* of O, then $\mathscr{D}(O) \cap O^\perp = \emptyset$. From uniqueness results for the Cauchy problem, see e.g. [**H4**, Section 28.4], one can get some geometric information on $\mathscr{D}(O)$. In particular, it was shown by Strohmaier in [**St**] that the *envelope* of O, see [**St**, Subsection 2.4] for the precise definition, is always included in $\mathscr{D}(O)$, provided the operator P is *locally analytic in time*. This condition means that near any point $x_0 \in M$, there exists local coordinates (t, x) such that ∂_t is time-like and the coefficients of P (and hence the metric g) are locally analytic in t.

Following Definition 6.1.1 we set

$$\mathcal{Y}(O) =: \frac{C_0^\infty(O)}{P(C_0^\infty(O))}, \text{ for } O \subset M \text{ open.}$$

PROPOSITION 6.2.2. *Let ω be a quasi-free state on* CCR(P) *with spacetime covariances $\Lambda^\pm$ and $O \subset M$ be open. Then $\mathcal{Y}(O)$ is dense in $\mathcal{Y}(\mathscr{D}(O))$ for the scalar product $\Lambda^+ + \Lambda^-$.*

Proof. Let $\mathcal{Y}^{\rm cpl}$ be the completion of $\mathcal{Y}$ for $\Lambda^+ + \Lambda^-$ and $A^\perp$ the orthogonal complement of $A \subset \mathcal{Y}^{\rm cpl}$. For $u \in \mathcal{Y}^{\rm cpl}$ we set

$$w_u^\pm(f) := \overline{u}\cdot\Lambda^\pm f, \quad f \in C_0^\infty(M).$$

Since $\Lambda^\pm \geq 0$, the Cauchy-Schwarz inequality yields

$$|w_u^\pm(f)| \leq (\overline{u}\cdot\Lambda^\pm u)^{\frac{1}{2}}(\overline{f}\cdot\Lambda^\pm f)^{\frac{1}{2}},$$

which implies that $w_u^\pm \in \mathcal{D}'(M)$. Moreover since $\Lambda^\pm P = 0$ we have $Pw_u^\pm = 0$. If $u \in \mathcal{Y}(0)^\perp$ we have $w_u^\pm = 0$ in O hence $w_u^\pm = 0$ in $\mathscr{D}(O)$ hence $u \in \mathcal{Y}(\mathscr{D}(O))^\perp$. □

Note that the density result in Proposition 6.2.2 is valid for *any* quasi-free state ω. It is hence different from the *Reeh-Schlieder property*, see Section 12.4, which is a property of a given state ω and asserts that $\mathcal{Y}(O)$ is dense in $\mathcal{Y}(O')$ for any open sets $O, O' \subset M$.

6.3. Conformal transformations

If (M, g) is globally hyperbolic and $c \in C^\infty(M)$ with $c(x) > 0$, then $(M, \tilde{g})$ for $\tilde{g} = c^2 g$ is also globally hyperbolic, with the same Cauchy surfaces as (M, g). It is easy to see from (5.4) that the Levi-Civita connection $\tilde{\nabla}$ for $\tilde{g}$ is given by:

$$\tilde{\nabla}_X Y = \nabla_X Y + c^{-1}\big((X\cdot dc)Y + (Y\cdot dc)X - X\cdot gY\nabla c\big). \tag{6.2}$$

If P is a Klein-Gordon operator on (M, g) and

$$W : L^2(M, dVol_{\tilde{g}}) \ni \tilde{u} \longmapsto c^{n/2-1}\tilde{u} \in L^2(M, dVol_g)$$

then

$$\tilde{P} := W^* P W = c^{-n/2-1} P c^{n/2-1}$$

is a Klein-Gordon operator on $(M, \tilde{g})$. In particular, if $P = -\Box_g + \frac{n-2}{4(n-1)}\mathrm{Scal}_g$ is the conformal wave operator for g, then $\tilde{P}$ is the conformal wave operator for $\tilde{g}$, see e.g. [**W1**, App. D].

Denoting with tildas the objects associated with $\tilde{g}$, $\tilde{P}$, we have:

$$G_{\rm ret/adv} = W\tilde{G}_{\rm ret/adv}W^*, \quad G = W\tilde{G}W^*. \tag{6.3}$$

6.3.1. Conformal transformations of phase spaces. Let us denote by $\tilde{M}$ the manifold M equipped with the density $dVol_{\tilde{g}} = c^n dVol_g$. If $\Sigma \subset M$ is a space-like Cauchy surface, then $\tilde{n} = c^{-1}n$, $\tilde{h} = c^2 h$. From (6.2) we obtain that $\nabla^{\tilde{A}} = W^{-1}\nabla^A W$. Let us set

$$U : C_0^\infty(\Sigma; \mathbb{C}^2) \ni f \longmapsto Uf = \begin{pmatrix} c^{1-n/2} f_0 \\ c^{-n/2} f_1 \end{pmatrix} \in C_0^\infty(\Sigma; \mathbb{C}^2).$$

The next proposition follows by easy computations.

PROPOSITION 6.3.1. *The following diagram is commutative, with all arrows unitary:*

$$\begin{array}{ccccc}
(\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\mathrm{i}G\,\cdot)_M) & \xrightarrow{G} & (\mathrm{Sol}_{\mathrm{sc}}(P), q) & \xrightarrow{\varrho_\Sigma} & (C_0^\infty(\Sigma;\mathbb{C}^2), q_\Sigma) \\
\big\downarrow W^* & & \big\downarrow W^{-1} & & \big\downarrow U \\
(\frac{C_0^\infty(\tilde{M})}{\tilde{P}C_0^\infty(\tilde{M})}, (\cdot\,|\mathrm{i}\tilde{G}\,\cdot)_{\tilde{M}}) & \xrightarrow{\tilde{G}} & (\mathrm{Sol}_{\mathrm{sc}}(\tilde{P}), \tilde{q}) & \xrightarrow{\tilde{\varrho}_\Sigma} & (C_0^\infty(\Sigma;\mathbb{C}^2), \tilde{q}_\Sigma)
\end{array}$$

6.3.2. Conformal transformations of quasi-free states. Let $\Lambda^\pm$ be the spacetime covariances of a quasi-free state ω for P. From (6.3) and Proposition 6.1.3 we obtain that

$$\tilde{\Lambda}^\pm = c^{1-n/2}\Lambda^\pm c^{-1-n/2} \tag{6.4}$$

are the spacetime covariances of a quasi-free state $\tilde{\omega}$ for $\tilde{P}$.

Let us denote by $\tilde{\Sigma}$ the manifold Σ equipped with the volume element $d\mathit{Vol}_{\tilde{h}}$. Then

$$U^*\tilde{f} = \begin{pmatrix} c^{n/2}\tilde{f}_0 \\ c^{n/2-1}\tilde{f}_1 \end{pmatrix},\ \tilde{f} \in C_0^\infty(\tilde{\Sigma};\mathbb{C}^2)$$

and

$$\tilde{\lambda}_\Sigma^\pm = (U^*)^{-1}\lambda_\Sigma^\pm U^{-1},$$

if $\lambda_\Sigma^\pm$, resp. $\tilde{\lambda}_\Sigma^\pm$ are the Cauchy surface covariances of ω, resp. $\tilde{\omega}$.

CHAPTER 7

Microlocal analysis of Klein-Gordon equations

The use of microlocal analysis in quantum field theory on curved spacetimes started with the fundamental papers of Radzikowski [**R1, R2**], who gave a definition of the *Hadamard states* by means of the *wavefront set* of their two-point functions, instead of their singularity structure, see e.g. Section 8.2. The work of Radzikowski relied on the analysis by Duistermaat and Hörmander [**DH**] of *distinguished parametrices* for Klein-Gordon operators, which was actually motivated by the desire to understand the notion of 'Feynman propagators' on curved spacetimes.

On Minkowski spacetime the interplay of microlocal analysis and quantum field theory is much older, see for example the proceedings [**P**].

In this chapter we first recall basic facts on wavefront sets of distributions on manifolds. We then describe the result of [**DH**] on distinguished parametrices and some related results due to Junker [**J1**].

7.1. Wavefront set of distributions

We recall the well-known definition of the *wavefront set* of a distribution $u \in \mathcal{D}'(M)$ for M a smooth manifold. We equip M with a smooth density, for which one usually takes $dVol_g$ if (M, g) is a spacetime. We use the notation $(\cdot|\cdot)_M$ in (5.9) for the duality bracket between $\mathcal{D}'(M)$ and $C_0^\infty(M)$.

Let $o \subset T^*M$ be the zero section. The points in $T^*M \setminus o$ will be denoted by $X = (x, \xi)$, $x \in M$, $\xi \in T_x^*M \setminus \{0\}$.

We recall that $\Gamma \subset T^*M \setminus o$ is *conic* if $(x, \xi) \in \Gamma \Rightarrow (x, \lambda\xi) \in \Gamma$ for all $\lambda > 0$. The *cosphere bundle* S^*M is the quotient of $T^*M \setminus o$ by the relation $X_1 \sim X_2$ if $x_1 = x_2$ and $\xi_1 = \lambda\xi_2$ for some $\lambda > 0$. A conic set Γ can be seen as a set in S^*M and it is called *closed* if it is closed in S^*M in the quotient topology.

Definition 7.1.1. *Let $\Omega \subset \mathbb{R}^n$ an open set. A point $(x_0, \xi_0) \in T^*\Omega \setminus o$ does not belong to the* wavefront set $\mathrm{WF}u$ *of $u \in \mathcal{D}'(\Omega)$ if there exist $\chi \in C_0^\infty(\Omega)$ with $\chi(x_0) = 1$ and a conic neighborhood Γ of ξ_0, such that*

$$|\mathcal{F}(\chi u)(\xi)| \leq C_N \langle\lambda\rangle^{-N}, \ \forall N \in \mathbb{N}, \ \xi \in \Gamma.$$

One can show that the wavefront set transforms covariantly under diffeomorphisms, i.e. if $\psi : \Omega_1 \xrightarrow{\sim} \Omega_2$ is a diffeomorphism, then

$$\mathrm{WF}(\psi^* u_2) = \psi^*(\mathrm{WF}(u_2)), \ \forall u_2 \in \mathcal{D}'(\Omega_2). \tag{7.1}$$

Another useful equivalent definition of $\mathrm{WF}u$ is as follows. We set

$$v_Y^\lambda(x) := \mathrm{e}^{\mathrm{i}\lambda(x-y)\cdot\eta}, \quad Y = (y, \eta) \in T^*\Omega, \quad x \in \mathbb{R}^n, \ \lambda \geq 1. \tag{7.2}$$

Lemma 7.1.2. *Let $\Omega \subset \mathbb{R}^n$ be an open set, $(x_0, \xi_0) \in T^*\Omega \setminus o$ and $u \in \mathcal{D}'(\Omega)$. Then $(x_0, \xi_0) \notin \mathrm{WF}u$ iff there exist $\chi \in C_0^\infty(\Omega)$ with $\chi(x_0) \neq 0$ and a neighborhood W of (x_0, ξ_0) in $T^*\Omega$ such that*

$$|(\chi v_Y^\lambda | u)_\Omega| \leq C_N \lambda^{-N}, \quad Y \in W, \ \lambda \geq 1, \ N \in \mathbb{N}.$$

From (7.1) we see that Definition 7.1.1 immediately extends to distributions on manifolds.

DEFINITION 7.1.3. *A point $X_0 = (x_0, \xi_0) \in T^*M \setminus o$ does not belong to the* wavefront set $\mathrm{WF}u$ *of $u \in \mathcal{D}'(M)$ if there exist a neighborhood U of x_0 and a chart diffeomorphism $\chi : U \xrightarrow{\sim} B(0,1)$ such that $(\chi^{-1})^* X_0 \notin \mathrm{WF}(\chi^{-1})^* u|_\Omega$.*

The wavefront set $\mathrm{WF}u$ is a closed conic subset of $T^*M \setminus o$ with $\pi_M \mathrm{WF}u = \operatorname{singsupp} u$, the *singular support of u*.

From Definition 7.1.3 we obtain immediately the *covariance property* of the wavefront set under diffeomorphisms.

PROPOSITION 7.1.4. *Let M_1, M_2 be two smooth manifolds and $\chi : M_1 \to M_2$ a diffeomorphism. Then*

$$\mathrm{WF}(\chi^* u_2) = \chi^*(\mathrm{WF}(u_2)) \ \forall\ u_2 \in \mathcal{D}'(M_2).$$

The following well-known result, see e.g. [**SVW**, Theorem 2.8], [**H1**, Theorem 8.4.8] allows to estimate the wavefront set of distributions defined as partial limits of holomorphic functions. It is usually expressed in terms of the *analytic wavefront set*, see Section 12.2.

PROPOSITION 7.1.5. *Let $I \subset \mathbb{R}$ be an open interval, S a smooth manifold and let $F : I \pm \mathrm{i}\,]0, \delta[\ni z \mapsto F(z) \in \mathcal{D}'(S)$ be a holomorphic function with values in $\mathcal{D}'(S)$. Assume that $f(t, \cdot) = \lim_{\epsilon \to 0^+} F(t \pm \mathrm{i}\epsilon, \cdot)$ exists in $\mathcal{D}'(I \times S)$. Then*

$$\mathrm{WF}(f) \subset \{(t, \tau) : t \in I,\ \pm\tau > 0\} \times T^*S.$$

Proof. We only prove the + case, and we can assume that $S = \Omega \subset \mathbb{R}^n$. We write $t = x^0$, $x = (x^0, x')$ for $x' \in S$ and $Y = (Y^0, Y')$ for $Y^0 \in T^*I$, $Y' \in T^*S$. With the notation in (7.2) we have $v_Y^\lambda(x) = v_{Y^0}^\lambda(x^0) v_{Y'}^\lambda(x')$. By Lemma 7.1.2, we need to show that

$$(v_Y^\lambda | \chi f)_{I \times S} \in O(\langle \lambda \rangle^{-\infty}), \ \text{uniformly for } Y \in W, \tag{7.3}$$

where $\chi^0 \in C_0^\infty(I)$, $\chi' \in C_0^\infty(S)$, $\chi(x) = \chi^0(x^0)\chi'(x')$ and $W \Subset \{Y \in T^*I \times S : \eta^0 < 0\}$ is relatively compact.

Arguing as in the proof of [**H1**, Theorem 3.1.14], we first obtain that if $K \Subset S$, there exist $N_0 \in \mathbb{N}$ and a semi-norm $\| \cdot \|_k$ of $C_0^\infty(K)$, such that

$$|(v | F(z, \cdot))_S| \leq C |\mathrm{Im} z|^{-N_0} \|v\|_k, \ \forall v \in C_0^\infty(K), \ z \in I + \mathrm{i}\,]0, \delta[\,.$$

For $v = \chi' v_{Y'}^\lambda$ we obtain:

$$|(\chi' v_{Y'}^\lambda | F(z, \cdot))_S| \leq C |\mathrm{Im} z|^{-N_0} \langle \lambda \rangle^k, \quad k \in \mathbb{N}, \ \text{uniformly for } Y' \in W' \Subset T^*S. \tag{7.4}$$

Let $\chi_1 \in C_0^\infty(\,]-\delta, \delta[\,)$ with $\chi_1 = 1$ in $|s| \leq \delta/2$ and

$$\tilde{\chi}^0(t + \mathrm{i}s) = \sum_{j=0}^N \partial_t^j \chi^0(t) \frac{(\mathrm{i}s)^j}{j!} \chi_1(s).$$

We have

$$\tilde{\chi}^0 \in C_0^\infty(\mathbb{C}), \quad \tilde{\chi}^0 \restriction_{\mathbb{R}} = \chi^0, \ \text{and } \partial_{\overline{z}} \tilde{\chi}^0 \in O(|\mathrm{Im} z|^N),$$

and $\tilde{\chi}^0$ is called an (N-th order) *almost analytic extension* of χ^0. Let us set

$$\overline{\varphi}_{Y^0}^\lambda(z) = \mathrm{e}^{-\frac{\lambda}{2}(z - x^0)^2 - \mathrm{i}\lambda(z - x^0)\xi^0},$$

which is holomorphic in $\mathbb{C}$ and equals $\overline{v_{Y^0}^\lambda}$ on $\mathbb{R}$. We apply Stokes formula

$$\int_\Omega \partial_{\overline{z}} g(z) d\overline{z} \wedge dz = \oint_{\partial\Omega} g(z) dz \tag{7.5}$$

to $g_Y^\lambda(z) = \overline{\varphi}_{Y^0}^\lambda(z)\tilde{\chi}^0(z)(\chi' v_{Y'}^\lambda | F(z,\cdot))_S$, $\Omega = \{\operatorname{Im} z > 0\}$. The right-hand side in (7.5) equals

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}} (\chi' v_{Y'}^\lambda | F(t+\mathrm{i}\epsilon,\cdot))_S \overline{\varphi}_{Y^0}^\lambda(t+\mathrm{i}\epsilon)\tilde{\chi}^0(t+\mathrm{i}\epsilon)dt = (\chi v_Y^\lambda | f)_{I\times S}.$$

Since $\partial_{\overline{z}} g_Y^\lambda(z) = \overline{\varphi}_{Y^0}^\lambda(z)(\chi' v_{Y'}^\lambda | F(z,\cdot))_S \frac{\partial\tilde{\chi}^0}{\partial\overline{z}}(z)$, we obtain using also (7.4) that the integrand in the lhs is bounded by $C|\mathrm{Im} z|^{N-N_0}\mathrm{e}^{-c\lambda|\mathrm{Im} z|}\langle\lambda\rangle^k$, uniformly for $Y \in W \Subset \{\eta^0 < 0\}$, $z \in \operatorname{supp}\tilde{\chi}^0$. Therefore the integral in the left-hand side is bounded by $C\langle\lambda\rangle^{k+N_0-N}$. Since N was arbitrary, we obtain (7.3). □

7.2. Operations on distributions

We refer the reader to [**H1**, Chap. 8].

7.2.1. Operations on conic sets. We first introduce some notation.
If $\Gamma \subset T^*M \setminus o$ is conic, we set

$$-\Gamma := \{(x,-\xi) :\ (x,\xi)\in\Gamma\},$$

and if $\Gamma_1, \Gamma_2 \subset T^*M \setminus o$ are conic, we set

$$\Gamma_1 + \Gamma_2 := \{(x, \xi_1+\xi_2) : (x,\xi_i)\in\Gamma_i\}.$$

Let M_i, $i = 1,2$ be two manifolds, o_i the zero section of T^*M_i, $M = M_1 \times M_2$, and let $\Gamma \subset T^*M \setminus o$ be a conic set. The elements of $T^*M \setminus o$ will be denoted by (x_1,ξ_1,x_2,ξ_2), which allows to consider Γ as a relation between T^*M_2 and T^*M_1, still denoted by Γ. Clearly Γ maps conic sets into conic sets. We set

$$\Gamma' := \{(x_1,\xi_1,x_2,-\xi_2) :\ (x_1,\xi_1,x_2,\xi_2)\in\Gamma\} \subset T^*(M_1\times M_2)\setminus o,$$

$$\mathrm{Exch}(\Gamma) := \Gamma^{-1} \subset (T^*M_2 \times T^*M_1)\setminus o,$$

$${}_{M_1}\Gamma := \{(x_1,\xi_1) :\ \exists\, x_2 \text{ such that } (x_1,\xi_1,x_2,0)\in\Gamma\} = \Gamma(o_2) \subset T^*M_1 \setminus o_1,$$

$$\Gamma_{M_2} := \{(x_2,\xi_2) :\ \exists\, x_1 \text{ such that } (x_1,0,x_2,\xi_2)\in\Gamma\} = \Gamma^{-1}(o_1) \subset T^*M_2 \setminus o_2.$$

7.2.2. Distribution kernels. If $M_i, i = 1,2$, are smooth manifolds equipped with smooth densities $d\mu_i$ and $K : C_0^\infty(M_2) \to \mathcal{D}'(M_1)$ is continuous, we will still denote by $K \in \mathcal{D}'(M_1\times M_2)$ its distribution kernel. Such a kernel is *properly supported* if the projection $\pi_2 : \operatorname{supp} K \to M_2$ is proper. If this is the case, then $K : C_0^\infty(M_2) \to \mathcal{E}'(M_1)$.

7.2.3. Complex conjugation and adjoints. If $u \in \mathcal{D}'(M)$, then

$$\mathrm{WF}(\overline{u}) = -\mathrm{WF}(u). \tag{7.6}$$

Similarly, if $K : C_0^\infty(M_2) \to \mathcal{D}'(M_1)$ is continuous and $K^* : C_0^\infty(M_1) \to \mathcal{D}'(M_2)$ is its adjoint with respect to some smooth densities $d\mu_1, d\mu_2$ then:

$$\mathrm{WF}(K^*)' = \mathrm{Exch}(\mathrm{WF}(K)'). \tag{7.7}$$

7.2.4. Pullback and restriction to submanifolds. Under a condition on $\mathrm{WF}u$ it is possible to extend the pullback $\chi^* u$ to general smooth maps $\chi : M_1 \to M_2$. Indeed, let us set $\chi^* u = u\circ\chi$ for $u \in C^\infty(M_2)$ and

$$N_\chi^* := \{(\chi(x_1),\xi_2) \in T^*M_2 \setminus o_2 :\ {}^tD\chi(x_1)\xi_2 = 0\}.$$

Then there is a unique extension of the *pullback* χ^* to distributions $u \in \mathcal{D}'(M_2)$ such that

$$N_\chi^* \cap \mathrm{WF}(u) = \emptyset, \tag{7.8}$$

and one has

$$\mathrm{WF}(\chi^* u) \subset \chi^* \mathrm{WF}(u). \tag{7.9}$$

In particular, if $S \subset M$ is a smooth submanifold and $i : S \to M$ is the canonical injection, the set N_i^* is denoted by N^*S and called the *conormal bundle* to S. One has:

$$N^*S = \{(x, \xi) \in T^*M : x \in S, \xi|_{T_x S} = 0\}.$$

The restriction $u\restriction_S = i^* u$ of $u \in \mathcal{D}'(M)$ is then well defined if

$$\mathrm{WF}u \cap N^*S = \emptyset, \tag{7.10}$$

and one has

$$\mathrm{WF}(u\restriction_S) \subset i^* \mathrm{WF}u. \tag{7.11}$$

7.2.5. Tensor products. If $u_i \in \mathcal{D}'(M_i)$ then

$$\begin{aligned} &WF(u_1 \otimes u_2) \\ \subset &(WF(u_1) \times WF(u_2)) \cup (\operatorname{supp} u_1 \times \{0\}) \times WF(u_2) \cup WF(u_1) \times (\operatorname{supp} u_2 \times \{0\}) \\ \subset &(WF(u_1) \times WF(u_2)) \cup o_1 \times WF(u_2) \cup WF(u_1) \times o_2. \end{aligned}$$

7.2.6. Products. The map $C_0^\infty(M)^2 \ni (u_1, u_2) \mapsto u_1 u_2$ uniquely extends to distributions $u_1, u_2 \in \mathcal{D}'(M)$ such that:

$$(\mathrm{WF}u_1 + \mathrm{WF}u_2) \cap o = \emptyset, \tag{7.12}$$

and one has

$$\mathrm{WF}(u_1 u_2) \subset \mathrm{WF}u_1 \cup \mathrm{WF}u_2 \cup (\mathrm{WF}u_1 + \mathrm{WF}u_2).$$

7.2.7. Kernels. If $K \in \mathcal{D}'(M_1 \times M_2)$, then the map $K : C_0^\infty(M_2) \to \mathcal{D}'(M_1)$ uniquely extends to distributions such that

$$u \in \mathcal{E}'(M_2), \quad \mathrm{WF}(u) \cap \mathrm{WF}(K)'_{M_2} = \emptyset, \tag{7.13}$$

and one has:

$$\mathrm{WF}(Ku) \subset {}_{M_1}\mathrm{WF}(K)' \cup (\mathrm{WF}(K)'(\mathrm{WF}u)), \tag{7.14}$$

where we interpret $\mathrm{WF}(K)'$ as a relation in $T^*M_1 \times T^*M_2$. Quite often one has ${}_{M_1}\mathrm{WF}(K)' = \emptyset$, and (7.14) simplifies to

$$\mathrm{WF}(Ku) \subset \mathrm{WF}(K)'(\mathrm{WF}u), \tag{7.15}$$

which justifies the use of $\mathrm{WF}(K)'$ instead of $\mathrm{WF}(K)$. Note for example that $\mathrm{WF}(Id)'$ is equal to the diagonal

$$\Delta = \{(X, X) : X \in T^*M \setminus o\} \tag{7.16}$$

which is the relation associated to $Id : T^*M \to T^*M$. Similarly, if P is a (properly supported) pseudodifferential operator (see Chapter 10) one has:

$$\mathrm{WF}(P)' \subset \Delta, \quad \text{hence } WF(Pu) \subset \mathrm{WF}(u),\ u \in \mathcal{D}'(M). \tag{7.17}$$

7.2.8. Composition of kernels. Finally, let $K_1 \in \mathcal{D}'(M_1 \times M_2)$, $K_2 \in \mathcal{D}'(M_2 \times M_3)$, where K_2 is properly supported. Then $K_1 \circ K_2$ is well defined if

$$\mathrm{WF}(K_1)'_{M_2} \cap {}_{M_2}\mathrm{WF}(K_2)' = \emptyset, \tag{7.18}$$

and then

$$\mathrm{WF}(K_1 \circ K_2)' \subset (\mathrm{WF}(K_1)' \circ \mathrm{WF}(K_2)') \cup ({}_{M_1}\mathrm{WF}(K_1)' \times o_3) \cup (o_1 \times \mathrm{WF}(K_2)'_{M_3}). \tag{7.19}$$

Again, it often happens that ${}_{M_i}\mathrm{WF}(K_i)'$ and $\mathrm{WF}(K_i)'_{M_{i+1}}$ are empty. Then (7.18) is automatic and (7.19) simplifies to the beautiful formula:

$$\mathrm{WF}(K_1 \circ K_2)' \subset \mathrm{WF}(K_1)' \circ \mathrm{WF}(K_2)'. \tag{7.20}$$

7.2.9. Proof of Proposition 6.1.6**.** We end this subsection by completing the proof of (2) in Proposition 6.1.6. Consider the map $\varrho_\Sigma^* G_\Sigma : C_0^\infty(\Sigma; \mathbb{C}^2) \to \mathcal{D}'(M)$. It is clearly continuous and introducing local coordinates (t, x) near $x_0 \in \Sigma$ such that $\Sigma = \{t = 0\}$ we see that

$$\mathrm{WF}(\varrho_\Sigma^* G_\Sigma)' \subset \{(X, Y) \in T^*M \times T^*\Sigma : X = i^*Y\},$$

where $i : \Sigma \to M$ is the canonical embedding. From $P \circ \Lambda^\pm = \Lambda^\pm \circ P = 0$ we obtain (see the proof of Lemma 7.4.3) that $\mathrm{WF}(\Lambda^\pm)' \subset \mathcal{N} \times \mathcal{N}$. Since Σ is space-like and hence non-null, we have $\mathcal{N} \cap N^*\Sigma = \emptyset$, which using Subsection 7.2.8 shows that $\Lambda^\pm \circ \varrho_\Sigma^* G_\Sigma : C_0^\infty(\Sigma; \mathbb{C}^2) \to \mathcal{D}'(M)$ is well defined and continuous. The same argument shows that $(\varrho_\Sigma^* G_\Sigma)^* \circ \Lambda^\pm \circ \varrho_\Sigma^* G_\Sigma : C_0^\infty(\Sigma; \mathbb{C}^2) \to \mathcal{D}'(\Sigma; \mathbb{C}^2)$ is well defined and continuous. □

7.3. Hörmander's theorem

We now state the famous result of Hörmander on propagation of singularities, see e.g. [**H3**, Theorem 26.1.1] or [**H4**, Theorem 3.2.1]. To this end we need some notions from *pseudodifferential calculus*, which will be recalled later on in Chapter 8.

The space of (classical) pseudodifferential operators of order m on a manifold X is denoted by $\Psi^m(X)$. If $P \in \Psi^m(X)$, its *principal symbol* $p = \sigma_{\mathrm{pr}}(P)$ is a smooth function on T^*X, homogeneous of degree m in ξ. Its *characteristic manifold* is

$$\mathrm{Char}(P) = p^{-1}(\{0\}) \setminus o,$$

where o is the zero section in T^*X. P is said of *real principal type* if p is real valued with $dp \neq 0$ on $\mathrm{Char}(P)$, which is then a smooth, conic hypersurface in T^*M, invariant under the flow of the Hamiltonian vector field H_p. The integral curves of H_p in $\mathrm{Char}(P)$ are traditionally called *bicharacteristic curves* for P. Note also that a Klein-Gordon operator P on a Lorentzian manifold (M, g) is of real principal type with principal symbol $p(x, \xi) = \xi \cdot g^{-1}(x)\xi$.

A submanifold $S \subset M$ is non-characteristic for P iff $\mathrm{Char}(P) \cap N^*S = \emptyset$.

THEOREM 7.3.1. *Let X be a smooth manifold and $P \in \Psi^m(X)$ a properly supported pseudodifferential operator. Then for $u \in \mathcal{D}'(X)$ one has:*

1. $\mathrm{WF}(u) \setminus \mathrm{WF}(Pu) \subset \mathrm{Char}(P)$ (microlocal ellipticity).
2. *If P is of real principal type, then $\mathrm{WF}(u) \setminus \mathrm{WF}(Pu)$ is invariant under the flow of H_p* (propagation of singularities).

7.4. The distinguished parametrices of a Klein-Gordon operator

We will recall some deep results of Duistermaat and Hörmander [**DH**] on *distinguished parametrices* of P. These results played a very important role in the work of Radzikowski [**R1**]. Let us first introduce some notation.

Recall that $C_\pm(x) \subset T_xM$ are the cones of future/past time-like vectors. We denote by $C_\pm(x)^* \subset T_x^*M$ the *dual cones*

$$C_\pm(x)^* = \{\xi \in T_x^*M : \ \xi \cdot v > 0, \ \forall v \in C_\pm(x), \ v \neq 0\}.$$

We write $\xi \rhd 0$ if $\xi \in C_+(x)^*$.

In this subsection P will be a Klein-Gordon operator on (M, g). We recall that its principal symbol is

$$\sigma_{\rm pr}(P)(x,\xi) = p(x,\xi) = \xi \cdot g^{-1}(x)\xi.$$

Duistermaat and Hörmander introduce in [**DH**] the *pseudo-convexity* condition of M with respect to P, which says that for any compact set $K \Subset M$ there exists a compact $K' \Subset M$ such that the projection on M of any bicharacteristic curve for P with endpoints in K is entirely contained in K'. Since projections on M of bicharacteristic curves are *null geodesics*, and hence causal curves, the pseudo-convexity of M follows easily from global hyperbolicity, using Lemma 5.4.3.

The characteristic manifold $\mathrm{Char}(P)$ will be denoted by $\mathcal{N}$; it splits into the *upper/lower energy shells*

$$\mathcal{N} = \mathcal{N}^+ \cup \mathcal{N}^-, \ \ \mathcal{N}^\pm = \mathcal{N} \cap \{\pm\xi \rhd 0\}. \tag{7.21}$$

Recall that $X = (x, \xi)$ denote the points in $T^*M \setminus o$. We write $X_1 \sim X_2$ if $X_1, X_2 \in \mathcal{N}$ and X_1, X_2 lie on the same integral curve of H_p.

For $X_1 \sim X_2$, we write $X_1 > X_2$, resp. $X_1 < X_2$ if $x_1 \in J_+(x_2)$, resp. $x_1 \in J_-(x_2)$ and $x_1 \neq x_2$ and we write $X_1 \succ X_2$, resp. $X_1 \prec X_2$ if X_1 comes strictly after, resp. before X_2 with respect to the natural parameter on the integral curve of H_p through X_1 and X_2. Finally, we set

$$\mathcal{C} = \{(X_1, X_2) \in \mathcal{N} \times \mathcal{N} : \ X_1 \sim X_2\},$$

and we introduce the following subsets of $\mathcal{C}$:

$$\begin{aligned}
&\mathcal{C}^\pm := \mathcal{C} \cap (\mathcal{N}^\pm \times \mathcal{N}^\pm),\\
&\mathcal{C}_{\rm ret} := \{(X_1, X_2) \in \mathcal{C} : \ X_1 > X_2\},\\
&\mathcal{C}_{\rm adv} := \{(X_1, X_2) \in \mathcal{C} : \ X_1 < X_2\},\\
&\mathcal{C}_{\rm F} := \{(X_1, X_2) \in \mathcal{C} : \ X_1 \prec X_2\},\\
&\mathcal{C}_{\overline{\rm F}} := \{(X_1, X_2) \in \mathcal{C} : \ X_1 \succ X_2\}.
\end{aligned} \tag{7.22}$$

Note that

$$\mathcal{C}_{\rm ret} \cup \mathcal{C}_{\rm adv} = \mathcal{C}_{\rm F} \cup \mathcal{C}_{\overline{\rm F}} = \mathcal{C} \setminus \Delta.$$

Using an orthogonal decomposition of the metric g, one easily obtains that

$$\begin{aligned}
\mathcal{C}_{\rm F} &= (\mathcal{C}_{\rm ret} \cap \mathcal{C}^+) \cup (\mathcal{C}_{\rm adv} \cap \mathcal{C}^-),\\
\mathcal{C}_{\bar{\rm F}} &= (\mathcal{C}_{\rm ret} \cap \mathcal{C}^-) \cup (\mathcal{C}_{\rm adv} \cap \mathcal{C}^+).
\end{aligned} \tag{7.23}$$

7.4.1. Parametrices.

Definition 7.4.1. *A continuous map $\tilde{G} : C_0^\infty(M) \to \mathcal{D}'(M)$ is a* left, *resp.* right parametrix *of P if*

$$\tilde{G} \circ P = \mathbb{1} + R, \ \textit{resp.} \ P \circ \tilde{G} = \mathbb{1} + R',$$

where R, resp. R' has a smooth kernel. If $\tilde{G}$ is both a left and a right parametrix, it is called a parametrix *of P.*

Parametrices play in microlocal analysis the role played by *pseudo-inverses* in Fredholm theory.

7.4.2. Distinguished parametrices. We now state a theorem of Duistermaat and Hörmander [**DH**, Theorem 6.5.3].

THEOREM 7.4.2. *For* $\sharp = \mathrm{ret}, \mathrm{adv}, \mathrm{F}, \overline{\mathrm{F}}$ *there exists a parametrix* $\tilde{G}_\sharp$ *of* P *such that*

$$\mathrm{WF}(\tilde{G}_\sharp)' = \Delta \cup \mathcal{C}_\sharp. \tag{7.24}$$

Any other left or right parametrix $\tilde{G}$ *with* $\mathrm{WF}(\tilde{G})' \subset \Delta \cup \mathcal{C}_\sharp$ *equals* $\tilde{G}_\sharp$ *modulo a smooth kernel.*

The parametrices in Theorem 7.4.2 are called *distinguished parametrices*. Those with $\mathrm{WF}(\tilde{G}') \subset \Delta \cup \mathcal{C}_{\mathrm{ret/adv}}$ are called *retarded/advanced parametrices*, while those with $\mathrm{WF}(\tilde{G}') \subset \Delta \cup \mathcal{C}_{\mathrm{F}/\overline{\mathrm{F}}}$ are called *Feynman/anti-Feynman parametrices*.

Note that the closed conic subsets Γ of $T^*(M \times M) \setminus o$ that can be equal to $\mathrm{WF}(\tilde{G})'$ for some parametrix $\tilde{G}$ of P were also completely characterized in [**DH**, Theorems 6.5.6, 6.5.8]. They can be very different from the sets in Theorem 7.4.2.

LEMMA 7.4.3. *The retarded/advanced inverses* $G_{\mathrm{ret/adv}}$ *introduced in Subsection 5.5.3 are advanced/retarded parametrices.*

Proof. We note first that since P is a differential operator, $P \otimes \mathbb{1}$ and $\mathbb{1} \otimes P$ are pseudodifferential operators on $M \times M$. Let now $\tilde{G}$ be a parametrix of P. We apply (7.17) and Theorem 7.3.1 (1) to $P \otimes \mathbb{1}$ or $\mathbb{1} \otimes P$, using the fact that $P \circ \tilde{G} - \mathbb{1}$ and $\tilde{G} \circ P - \mathbb{1}$ have smooth kernels, and obtain that

$$\Delta \subset \mathrm{WF}(\tilde{G})' \subset (\mathcal{N} \times \mathcal{N}) \cup \Delta.$$

Let us assume now that there exists $(X_1, X_2) \in \mathrm{WF}(G_{\mathrm{ret}})'$ with $(X_1, X_2) \notin \Delta \cup \mathcal{C}_{\mathrm{ret}}$. If $X_1 \sim X_2$, then necessarily $x_1 \notin J_+(x_2)$, hence $(x_1, x_2) \notin \mathrm{supp}\, G_{\mathrm{ret}}$, which is a contradiction. If $X_1 \not\sim X_2$, then necessarily $X_1, X_2 \in \mathcal{N}$. If $B(X)$ denotes the bicharacteristic curve through X, then $B(X_1) \times \{X_2\} \cap \Delta = \emptyset$. We can apply then Theorem 7.3.1 (2) to $P \otimes \mathbb{1}$, using that $P \circ G_{\mathrm{ret}} - \mathbb{1}$ has a smooth kernel, to obtain that $B(X_1) \times \{X_2\} \subset \mathrm{WF}(G_{\mathrm{ret}})'$. In particular, $\mathrm{WF}(G_{\mathrm{ret}})'$ contains (X_3, X_2) with $x_3 \notin J_+(x_2)$, which is a contradiction. The proof for G_{adv} is similar. □

By Lemma 7.4.3, there are canonical advanced/retarded parametrices, namely the advanced/retarded inverses. No such canonical choice exists of Feynman/anti-Feynman inverses, at least on general spacetimes (M, g), a fact already noted by Duistermaat and Hömander. This fact is related to the absence of a canonical choice of *Hadamard states* for P, see Chapter 8 below. We will come back to this question in Chapter 16.

We end this subsection with a proposition about the wavefront set of *differences* of distinguished parametrices, due to Junker, see [**J1**, Theorem 2.29].

PROPOSITION 7.4.4. *One has:*

(1) $\mathrm{WF}(\tilde{G}_{\mathrm{ret}} - \tilde{G}_{\mathrm{adv}})' = \mathcal{C}$,

(2) $\mathrm{WF}(\tilde{G}_{\mathrm{F}} - \tilde{G}_{\overline{\mathrm{F}}})' = \mathcal{C}$,

(3) $\mathrm{WF}(\tilde{G}_{\mathrm{F}} - \tilde{G}_{\mathrm{ret}})' = \mathcal{C}^-$,

(4) $\mathrm{WF}(\tilde{G}_{\mathrm{F}} - \tilde{G}_{\mathrm{adv}})' = \mathcal{C}^+$.

Proof. We will apply the following observation: let S be any of the differences in Proposition 7.4.4. Since $PS, SP \in C^\infty(M \times M)$, applying Theorem 7.3.1 to $P \otimes \mathbb{1}$ and $\mathbb{1} \otimes P$ we obtain that

$$\begin{aligned} &\text{(i)} \quad \mathrm{WF}S' \subset \mathcal{N} \times \mathcal{N}, \\ &\text{(ii)} \quad (X_1, X_2) \in (\mathcal{N} \times \mathcal{N}) \setminus \mathrm{WF}S' \Rightarrow B(X_1) \times B(X_2) \cap \mathrm{WF}S' = \emptyset, \end{aligned} \tag{7.25}$$

where we recall that $B(X)$ is the bicharacteristic curve through X. In the sequel we set $\Delta_{\mathcal{N}} = (\mathcal{N} \times \mathcal{N}) \cap \Delta$.

Let us prove assertion (1). Since $\mathrm{WF}(\tilde{G}_{\mathrm{ret}})' \setminus \Delta_{\mathcal{N}}$ and $\mathrm{WF}(\tilde{G}_{\mathrm{adv}})' \setminus \Delta_{\mathcal{N}}$ are disjoint, we obtain that

$$\mathrm{WF}(\tilde{G}_{\mathrm{ret}} - \tilde{G}_{\mathrm{adv}})' \setminus \Delta_{\mathcal{N}} = \Big(\mathrm{WF}(\tilde{G}_{\mathrm{ret}})' \setminus \Delta_{\mathcal{N}}\Big) \cup \Big(\mathrm{WF}(\tilde{G}_{\mathrm{adv}})' \setminus \Delta_{\mathcal{N}}\Big) = \mathcal{C} \setminus \Delta_{\mathcal{N}}. \tag{7.26}$$

Next, (7.25) (i) implies that $\mathrm{WF}(\tilde{G}_{\mathrm{ret}} - \tilde{G}_{\mathrm{adv}})' \subset \mathcal{N} \times \mathcal{N}$, and (7.25) (ii) combined with (7.26) implies that $\Delta_{\mathcal{N}} \subset \mathrm{WF}(\tilde{G}_{\mathrm{ret}} - \tilde{G}_{\mathrm{adv}})'$. This completes the proof of (1). The proof of (2) is similar.

Now let us prove (3). Since $\mathrm{WF}(G_{\mathrm{ret}})' \cap \{(X_1, X_2) \in \mathcal{N} \times \mathcal{N} : X_1 < X_2\} = \emptyset$, we have:

$$\begin{aligned} & \mathrm{WF}(\tilde{G}_{\mathrm{F}} - \tilde{G}_{\mathrm{ret}})' \cap \{(X_1, X_2) \in \mathcal{N} \times \mathcal{N} : X_1 < X_2\} \\ = \ & \mathrm{WF}\tilde{G}'_{\mathrm{F}} \cap \{(X_1, X_2) \in \mathcal{N} \times \mathcal{N} : X_1 < X_2\} \\ = \ & \mathcal{C}_{\mathrm{F}} \cap \mathcal{C}_{\mathrm{adv}} = \mathcal{C}_{\mathrm{adv}} \cap \mathcal{C}^-, \end{aligned} \tag{7.27}$$

where in the last step we used (7.23). Applying then (7.25) we obtain (3). The proof of (4) is similar. □

CHAPTER 8

Hadamard states

The main problem one encounters when considering quantum Klein-Gordon fields on a curved spacetime is that there is no notion of a *vacuum state*. Unless the spacetime is stationary, see Chapter 9, there is no one-parameter group of Killing isometries that can be used to define a vacuum state.

One is forced to find a more general class of physically acceptable states, which should be those for which the *renormalized stress-energy tensor* $T_{ab}(\phi)(x)$, see Section 8.1, can be rigorously defined. Alternatively one can require that the short distance behavior of their two-point functions, expressed for example in normal coordinates at any point $x \in M$, should mimic the one of the vacuum state on Minkowski spacetime.

These states are called *Hadamard states* and play a fundamental role in quantum field theory on curved spacetimes. In this chapter we describe the characterization of Hadamard states due to Radzikowski, **[R1, R2]**, relying on the wavefront set of their two-point functions and various existence and uniqueness theorems for Hadamard states. The microlocal definition of Hadamard states is very convenient and natural for applications.

8.1. The need for renormalization

Let us now consider a *non-linear* Klein-Gordon equation like

$$-\Box_g\phi(x) + m^2\phi(x) + \phi^n(x) = 0, \tag{8.1}$$

or a Klein-Gordon equation coupled to another classical field equation, like the *Einstein Klein-Gordon system*:

$$\begin{cases} R_{\mu\nu}(g) - \frac{1}{2}R(g)g_{\mu\nu} = T_{\mu\nu}(\phi), \\ -\Box_g\phi + m^2\phi = 0. \end{cases} \tag{8.2}$$

Here $T_{ab}(\phi)$ is the *stress-energy tensor* of ϕ, defined as

$$T_{ab}(\phi) = \nabla_a\phi\nabla_b\phi - \frac{1}{2}g_{ab}(\nabla^c\phi\nabla_c\phi + m^2\phi^2), \tag{8.3}$$

for a real solution ϕ. For complex solutions the stress-energy tensor is defined as

$$T_{ab}(\phi) = \overline{\nabla_a\phi}\nabla_b\phi + \overline{\nabla_b\phi}\nabla_a\phi - g_{ab}(\overline{\nabla^c\phi}\nabla_c\phi + m^2\overline{\phi}\phi). \tag{8.4}$$

Note that if $\phi \in C^\infty(M)$ solves the Klein-Gordon equation

$$-\Box_g\phi + V(x)\phi = 0,$$

then one has the identity

$$\nabla^a T_{ab}(\phi) = (V - m^2)(\overline{\phi}\nabla_b\phi + \overline{\nabla_b\phi}\phi), \tag{8.5}$$

(this vanishes if $V = m^2$), which is the basic ingredient of *energy estimates* for Klein-Gordon equations.

To quantize such classical equations, one would like to define expressions like $\phi^n(x)$, or $T_{ab}(\phi)(x)$ as operator-valued distributions.

It is hopeless to define $\int_M \phi^n(x)u(x)dVol_g$ or $\int_M T_{ab}(\phi)(x)u(x)dVol_g$ for $u \in C_0^\infty(M)$ as elements of an abstract $*$-algebra.

Instead one can hope that given a state ω for the *free* Klein-Gordon field, those expressions may have a meaning as unbounded operators on the GNS Hilbert space $\mathcal{H}_\omega$. More precisely one can try to proceed as follows:

Let $\phi_\omega(u)$ for $u \in C_0^\infty(M)$, be the image of the abstract field $\phi(u)$ under the map π_ω of the GNS triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, and let $\phi_\omega(x)$ be the operator-valued distribution on M defined by $\phi_\omega(u) =: \int_M \phi_\omega(x)u(x)dVol_g$. Then one can try to define

$$\phi^2_\omega(x) = \lim_{x' \to x} \phi_\omega(x)\phi_\omega(x'),$$

i.e. $\phi^2_\omega(x)$ will be the trace on the diagonal $\Delta = \{x = x'\}$ of the operator valued distribution $\phi_\omega(x)\phi_\omega(x')$ on $M \times M$. If this is possible, then one would expect that $(\Omega_\omega|\phi^2_\omega(x)\Omega_\omega)_{\mathcal{H}_\omega}$ will be a well-defined (scalar) distribution on M. In the Minkowski case this means that the two-point function $\omega_2(x, x')$ has a well-defined trace on Δ. This is clearly impossible, since by (3.14)

$$\omega_2(x, x) = \int_{\mathbb{R}^d} \epsilon(\mathrm{k})^{-1} d\mathrm{k} = \infty,$$

an example of *ultraviolet divergence*. Note also that one has

$$\mathrm{WF}(\omega_2) = \{((x, \xi), (x', \xi')) : (x, \xi) \in \mathcal{N}^+, (x', \xi') \in \mathcal{N}^-, (x, \xi) \sim (x', -\xi')\}, \tag{8.6}$$

so trying to define $\omega_2|_\Delta$ by the arguments of Section 7.2 does not work either.

8.1.1. The Wick ordering. The solution to this problem for the vacuum state on Minkowski is well-known, and called the *Wick ordering*: it consists in setting

$$:\phi(x)\phi(x'):= \phi(x)\phi(x') - \omega_2(x, x')\mathbb{1}. \tag{8.7}$$

If ω is any quasi-free state, then $:\phi_\omega(x)\phi_\omega(x'):$ is clearly well defined as an operator-valued distribution on $M \times M$. If $\omega = \omega_{\mathrm{vac}}$, let us try to define the operator-valued distribution: $\phi^2_{\omega_{\mathrm{vac}}}(x)$: as the trace on Δ of $:\phi_{\omega_{\mathrm{vac}}}(x)\phi_{\omega_{\mathrm{vac}}}(x'):$. To this end, we consider the distribution

$$\begin{aligned} &:\phi_\omega(x)\phi_\omega(x'): \times :\phi_\omega(y)\phi_\omega(y'):= \phi_\omega(x)\phi_\omega(x')\phi_\omega(y)\phi_\omega(y') \\ - \quad &\phi_\omega(x)\phi_\omega(x')\omega_2(y, y') - \phi_\omega(y)\phi_\omega(y')\omega_2(x, x') + \omega_2(x, x')\omega_2(y, y')\mathbb{1}. \end{aligned}$$

Using the fact that ω is quasi-free, see Proposition 4.6.4, we obtain that

$$\omega\big(:\phi_\omega(x)\phi_\omega(x'): \times :\phi_\omega(y)\phi_\omega(y'):\big) = \omega_2(x, y)\omega_2(x', y') + \omega_2(x, y')\omega_2(x', y).$$

The right-hand side above has a well-defined trace on $\{x = x', y = y'\}$, which equals $2\omega_2(x, y)^2$. Note that $\omega_2(x, y)^2$ is well defined as an element of $\mathcal{D}'(M \times M)$, since if Γ is the right-hand side in (8.6) we have $(\Gamma + \Gamma) \cap o = \emptyset$.

Summarizing we have shown that the vector

$$\int_M :\phi^2(x): u(x)dVol_g\Omega_\omega, \quad u \in C_0^\infty(M)$$

is well defined as an element of $\mathcal{H}_\omega$ for $u \in C_0^\infty(M)$ (since its norm in $\mathcal{H}_\omega$ is finite). Using the same argument one can show that the (unbounded) operator $\int_M :\phi^2(x): u(x)dVol_g$ is well defined with domain

$$\mathcal{D} = \mathrm{Vect}\{\prod_{i=1}^n \phi_\omega(u_i)\Omega_\omega : u_i \in C_0^\infty(M), n \in \mathbb{N}\}.$$

8.2. Old definition of Hadamard states

The Wick ordering is well understood for the Klein-Gordon field on Minkowski spacetime. The search for a natural class of *vacuum states* for Klein-Gordon fields on more general globally hyperbolic spacetimes led physicists to introduce the notion of *Hadamard states*.

Originally, Hadamard states were defined by specifying the singularity of their two-point functions $\omega_2(x,x') = \omega(\phi(x)\phi(x'))$ for pair of points $(x,x') \in M \times M$ near the diagonal, see e.g. [**KW**, Section 3.3].

We will follow here the exposition of Radzikowski in [**R1**, Section 5], see also the PhD thesis of Viet Dang [**D**, Sections 5.2, 5.3].

Let us first consider the Minkowski case and set $Q(x) = x\cdot\eta x$ for $x \in \mathbb{R}^n$. We first claim that

$$Q(x+\mathrm{i}y) \in \mathbb{C}\setminus\,]-\infty,0], \quad x \in \mathbb{R}^n, y \in C, \tag{8.8}$$

where we recall from Section 2.1 that $C = C_+ \cup C_- \subset \mathbb{R}^n$ is the cone of time-like vectors. Indeed we have

$$Q(x+\mathrm{i}y) = x\cdot\eta x - y\cdot\eta y + 2\mathrm{i}x\cdot\eta y.$$

If $\operatorname{Im} Q(x+\mathrm{i}y) = 0$ and $y \in C$, then x is space-like by Lemma 5.2.3, hence $\operatorname{Re} Q(x+\mathrm{i}y) > 0$, which proves our claim. Moreover, if $\Gamma \Subset C_+$ is a closed cone and $K \Subset \mathbb{R}^n$ is compact, then there exist $\delta > 0$ and $R > 0$ such that

$$|Q(x+iy)| \geq \delta|y|^2, \quad \forall x \in K, y \in \Gamma \cap \{|y| \leq R\}. \tag{8.9}$$

Writing

$$|Q(x+iy)|^2 = (x\cdot\eta x - y\cdot\eta y)^2 + 4(x\cdot\eta y)^2,$$

we see that (8.9) is clearly satisfied for $x \in K, x\cdot\eta x \geq 0$ and $y \in \Gamma$, since $-y\cdot\eta y \geq c|y|^2$ for $y \in \Gamma$. If $x\cdot\eta x < 0$, $x \in K$, then from Lemma 5.2.3 we obtain that $|x\cdot\eta y| \geq c|y|$ for $y \in \Gamma$. This implies (8.9).

In the sequel we take the determination of $\log z$ which is defined in $\mathbb{C}\setminus\,]-\infty,0]$. It follows from (8.8), (8.9) that $Q^{-1}(z), \log Q(z)$ are holomorphic functions of *moderate growth* in $\mathbb{R}^n + \mathrm{i}C_+$, see Section 12.1, hence the boundary values

$$(Q^{-1})_+(x) := Q^{-1}(x+\mathrm{i}C_+0), \quad (\log Q)_+(x) := \log Q(x+\mathrm{i}C_+0) \tag{8.10}$$

are well defined as distributions on $\mathbb{R}^n$.

The limit in (8.10) can be taken in particular along any vector $y \in C_+$, see Subsection 12.1.2, which implies that the distributions $(Q^{-1})_+$ and $(\log Q)_+$ are invariant under the action of the restricted Lorentz group $SO^\uparrow(1,d)$.

Now let (M,g) be a spacetime. There exists a neighborhood U of the zero section in TM such that the map:

$$\exp : U \ni (x,v) \longmapsto (x, \exp^g_x(v)) \in M \times M$$

is a diffeomorphism onto its range, with $V = \exp(U)$ being a neighborhood of the diagonal Δ in $M \times M$. Clearly, such sets V form a basis of neighborhoods of Δ.

Let us also fix a smooth map

$$R : M \ni x \longmapsto R(x) \in L(T_xM, \mathbb{R}^n)$$

such that $R(x) : (T_xM, g(x)) \to (\mathbb{R}^n, \eta)$ is pseudo-orthogonal and maps the future lightcone $C_+(x)$ into C_+, i.e. preserves the time orientation. One can then define the map

$$F : V \ni (x,x') \longmapsto R(x') \circ (\exp^g_{x'})^{-1}(x) \in \mathbb{R}^n, \tag{8.11}$$

which has a surjective differential. Note that $Q \circ F(x,x')$ equals the (signed) *square geodesic distance* $\sigma(x,x')$ between x and x'. Since $N_F^* = \emptyset$, we can by Subsection 7.2.4 define the pullbacks of $(Q^{-1})_+$ and $(\log Q)_+$ by F

$$(\sigma^{-1})_+ := F^*((Q^{-1})_+), \quad \text{and} \quad (\log\sigma)_+ := F^*((\log Q)_+) \in \mathcal{D}'(V).$$

From the invariance of $(Q^{-1})_+$ and $(\log Q)_+$ under $SO^\uparrow(1,d)$, we deduce that $(\sigma^{-1})_+$ and $(\log\sigma)_+$ are independent of the choice of $R(x)$.

One defines also the *van Vleck-Morette determinant*

$$\Delta(x,x') := -\det(-\nabla_\alpha \nabla_{\beta'}\sigma(x,x'))|g|^{-\frac{1}{2}}(x)|g|^{-\frac{1}{2}}(x').$$

Definition 8.2.1. *Let P be a real Klein-Gordon operator. A quasi-free state ω on $\mathrm{CCR}_{\mathbb{R}}(P)$ is a* Hadamard state *if there exist a neighborhood V of the diagonal in $M \times M$ as above and functions $v, w \in C^\infty(V)$, such that*

$$\begin{aligned} \omega_{2\mathbb{C}}(x,x') = \ & \tfrac{1}{(2\pi)^2}\Delta^{\frac{1}{2}}(x,x')(\sigma^{-1})_+(x,x') \\ & + v(x,x')(\log\sigma)_+(x,x') + w(x,x') \quad \text{on } V. \end{aligned} \tag{8.12}$$

Note that the function $v(x,x')$ is not arbitrary, since $P_x\omega_2 = P_{x'}\omega_2 = 0$. One has

$$v(x,x') \sim \sum_{i=0}^{\infty} v_i(x,x')\sigma(x,x')^i,$$

where $v_i(x,x')$ are the so-called *Hadamard coefficients* and the $\sim$ symbol means that

$$v - \sum_{i=0}^{n} v_i\sigma^i \in O(|\sigma|^{n+1}),\ \forall n \in \mathbb{N}$$

together with all derivatives.

8.3. The microlocal definition of Hadamard states

The situation was radically simplified by Radzikowski, who in [**R1**] introduced the definition of a Hadamard state via the *wavefront set* of its two-point function. Let us first introduce the original definition, which deals with *real fields*, see Subsection 6.1.3.

8.3.1. Hadamard condition for real fields. We use the notation for real Klein-Gordon fields recalled in Subsection 6.1.3.

Definition 8.3.1. *Let ω be a quasi-free state on $\mathrm{CCR}_{\mathbb{R}}(P)$, with real covariance H. Then ω is a* Hadamard state *if*

$$\mathrm{WF}(\omega_{2\mathbb{C}})' = \{(X,X') \in T^*M \times T^*M : X, X' \in \mathcal{N}^+, X \sim X'\}. \tag{8.13}$$

8.3.2. The Hadamard condition for complex fields. As already explained in Chapter 4, it is much more convenient to work with complex fields and gauge invariant states, i.e. in the framework of Chapter 6. In this case the following definition was introduced in [**GW1**].

Definition 8.3.2. *Let ω be a (gauge invariant) quasi-free state, with spacetime covariances $\Lambda^\pm : C_0^\infty(M) \to \mathcal{D}'(M)$. Then ω is a* Hadamard state *if*

$$\mathrm{WF}(\Lambda^\pm)' = \{(X,X') \in T^*M \times T^*M : X, X' \in \mathcal{N}^\pm, X \sim X'\}.$$

8.4. The theorems of Radzikowski

We now prove the theorems of Radzikowski [**R1, R2**] on the microlocal characterization of Hadamard states. We will use the formalism of complex fields, in which case Theorem 8.4.2 is due to Wrochna [**W1**].

Let us first introduce a list of conditions.

DEFINITION 8.4.1. *A pair of continuous maps* $\Lambda^\pm : C_0^\infty(M) \to \mathcal{D}'(M)$ *satisfy*

(Herm) *if* $\Lambda^\pm - \Lambda^{\pm *} = 0$ *modulo* C^∞;

(Pos) *if* $\Lambda^\pm \geq 0$ *modulo* C^∞;

(CCR) *if* $\Lambda^+ - \Lambda^- = \mathrm{i}G$ *modulo* C^∞;

(KG) *if* $P\Lambda^\pm = \Lambda^\pm P = 0$ *modulo* C^∞;

(Had) *if* $\mathrm{WF}(\Lambda^\pm)' = \{(X, X') \in T^*M \times T^*M : X, X' \in \mathcal{N}^\pm, X \sim X'\}$;

(genHad) *if* $\mathrm{WF}(\Lambda^\pm)' \subset \{X : \pm\xi \rhd 0\} \times \{X : \pm\xi \rhd 0\}$;

(genHadloc) *if* $\mathrm{WF}(\Lambda^\pm)' \cap \Delta \subset \{(X, X) : \pm\xi \rhd 0\}$;

(Feynm) *if* $\mathrm{i}^{-1}\Lambda^+ + G_{\mathrm{adv}}$, $\mathrm{i}^{-1}\Lambda^- + G_{\mathrm{ret}}$ *are Feynman parametrices of* P.

THEOREM 8.4.2. *The following conditions are equivalent:*

(1) $\Lambda^\pm$ *satisfy* (Had), (KG), (CCR)*;*
(2) $\Lambda^\pm$ *satisfy* (genHad), (KG), (CCR)*;*
(3) $\Lambda^\pm$ *satisfy* (Feynm).

Proof. (1)$\Longrightarrow$ (2) is obvious. Let us prove the implication (2)$\Longrightarrow$(3). Let $\tilde{G}_{\mathrm{F}}$ be a Feynman parametrix of P. If $S^\pm = \mathrm{i}(\tilde{G}_{\mathrm{F}} - G_{\mathrm{adv/ret}})$ we have $\mathrm{WF}(S^\pm)' \subset \mathcal{C}^\pm$, by Proposition 7.4.4 and $\mathrm{WF}(\Lambda^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm$ by (genHad) and Theorem 7.3.1. Hence, $\mathrm{WF}(\Lambda^\pm - S^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm$ and

$$\mathrm{WF}(\Lambda^+ - S^+)' \cap \mathrm{WF}(\Lambda^- - S^-)' = \emptyset.$$

On the other hand, by (CCR) we obtain

$$(\Lambda^+ - S^+) - (\Lambda^- - S^-) = (\Lambda^+ - \Lambda^-) - (S^+ - S^-) = \mathrm{i}G - \mathrm{i}G = 0.$$

Therefore, $S^\pm - \Lambda^\pm$ has a smooth kernel, which implies (3).

Finally we prove that (3)$\Longrightarrow$(1). (KG) and (CCR) are immediate and (Had) follows from Proposition 7.4.4. □

Since the spacetime covariances $\Lambda^\pm$ of a Hadamard state satisfy (CCR), (KG) and (Had), we immediately obtain the following corollary, which says that these covariances are unique, modulo smooth kernels.

COROLLARY 8.4.3. *Let* $\Lambda_i^\pm$, $i = 1, 2$ *be the spacetime covariances of two Hadamard states* ω_i*. Then* $\Lambda_1^\pm - \Lambda_2^\pm$ *have smooth kernels.*

Another important result is the following theorem, due to Duistermaat and Hörmander [**DH**, Theorem 6.6.2] in a more general context. The proof we give follows from the *existence* of Hadamard states, see Section 8.7.

THEOREM 8.4.4. (Feynm) *implies* (Pos).

Proof. We know from Thm 8.9.1 that Hadamard states for P exist. Let $\Lambda_1^\pm$ be the spacetime covariances of a Hadamard state for P, which satisfy (Had), (KG) and (CCR), hence (Feynm). If $\Lambda^\pm$ satisfy also (Feynm), then $\Lambda^\pm - \Lambda_1^\pm$ have smooth kernels. Since $\Lambda_1^\pm \geq 0$, $\Lambda^\pm$ satisfy (Pos). □

Finally we prove a variant of a result of Radzikowski [**R2**] called there a 'local-to-global theorem'.

PROPOSITION 8.4.5. (Pos) *and* (genHadloc) *imply* (genHad).

The proof follows immediately from Lemma 8.4.6 below.

LEMMA 8.4.6. *Let $K \in \mathcal{D}'(M \times M)$ such that $K \geq 0$ modulo a smooth kernel. Then for $X \in T^*M \setminus o$ we have*

$$(X, X) \notin \mathrm{WF}(K)' \Rightarrow (X_1, X), (X, X_2) \notin \mathrm{WF}(K)',\ \forall X_i \in T^*M \setminus o.$$

Proof. We may assume that $K \geq 0$ and that $M = \Omega \subset \mathbb{R}^n$. Let v_Y^λ be defined in (7.2). We see that $(X_1, X_2) \notin \mathrm{WF}(K)'$ iff there exists $\chi_i \in C_0^\infty(M)$ with $\chi_i(x_i) \neq 0$ and neighborhoods $W_i \Subset T^*M$ of X_i such that

$$(\chi_1 v_{Y_1}^\lambda | K \chi_2 v_{Y_2}^\lambda)_M \in O(\langle\lambda\rangle^{-\infty}),\ \text{ uniformly for } Y_i \in W_i.$$

Note also that since $K : C_0^\infty(M) \to \mathcal{D}'(M)$ is continuous, we have

$$|(\chi v_Y^\lambda | K \chi v_Y^\lambda)_M| \leq C\langle\lambda\rangle^{N_0} \text{ uniformly for } Y \in W \Subset T^*M,$$

for some N_0 depending on χ, W. By the Cauchy-Schwarz inequality, we obtain

$$|(\chi_1 v_{Y_1}^\lambda | K \chi_2 v_{Y_2}^\lambda)_M| \leq (\chi_1 v_{Y_1}^\lambda | K \chi_1 v_{Y_1}^\lambda)_M^{\frac{1}{2}} (\chi_1 v_{Y_2}^\lambda | K \chi_2 v_{Y_2}^\lambda)_M^{\frac{1}{2}},$$

which yields the lemma. □

8.5. The Feynman inverse associated to a Hadamard state

Let ω a Hadamard state with spacetime covariances $\Lambda^\pm$. Then

$$G_{\mathrm{F}} := \mathrm{i}^{-1}\Lambda^+ + G_{\mathrm{adv}} = \mathrm{i}^{-1}\Lambda^- + G_{\mathrm{ret}} \tag{8.14}$$

is a *Feynman inverse* of P, i.e. one has

$$PG_{\mathrm{F}} = G_{\mathrm{F}}P = \mathbb{1}, \quad \mathrm{WF}(G_{\mathrm{F}})' = \Delta \cup C_{\mathrm{F}}.$$

The operator G_{F} will be called the *Feynman inverse* associated to ω.

8.6. Conformal transformations

We use the notation in Section 6.3. Let ω be a quasi-free state for P and $\tilde{\omega}$ the associated quasi-free state for $\tilde{P}$ obtained from (6.4), where we recall that $\tilde{P} = c^{-n/2-1} P c^{n/2-1}$ and $\tilde{g} = c^2 g$.

Clearly, $\tilde{\omega}$ is Hadamard iff ω is Hadamard.

8.7. Equivalence of the two definitions

In this subsection we prove the equivalence of Definition 8.2.1 and Definition 8.3.1, following **[R1]**.

THEOREM 8.7.1. *A quasi-free state ω for a real Klein-Gordon operator P satisfies Definition* 8.2.1 *iff it satisfies Definition* 8.3.1.

Proof. Let $\Lambda^\pm$ the complex covariances of the complexification of the state ω_2, see Subsection 4.7.2. By (4.26) we have

$$\Lambda^+ = \omega_{2\mathbb{C}}, \quad \Lambda^- = \omega_{2\mathbb{C}} - \mathrm{i}G_{\mathbb{C}} = {}^t\omega_{2\mathbb{C}},$$

since $\omega_{2\mathbb{C}} - {}^t\omega_{2\mathbb{C}} = \mathrm{i}G_{\mathbb{C}}$, see Proposition 6.1.7. Note that if $K : C_0^\infty(M) \to \mathcal{D}'(M)$ we have $\mathrm{WF}({}^tK)' = -\mathrm{WF}(K)'$. Assume that $\omega_{2\mathbb{C}}$ satisfies (8.12). By Proposition 8.7.2, $\omega_{2\mathbb{C}}$ satisfies (genHadloc), hence (genHad) by Proposition 8.4.5. By the above remark, $\Lambda^\pm$ satisfy (genHad), and of course (CCR) and (KG). By Theorem 8.4.2, we obtain that $i^{-1}\omega_{2\mathbb{C}} + G_{\mathrm{adv}}$ is a Feynman parametrix for P, hence $\omega_{2\mathbb{C}}$ satisfies (8.13), again by Theorem 8.4.2.

Conversely, if $\omega_{2\mathbb{C}}$ satisfies (8.13), then by the same argument $i^{-1}\omega_{2\mathbb{C}} + G_{\rm adv}$ is a Feynman parametrix for P, hence satisfies (8.12) by the above discussion and the uniqueness of Feynman parametrices modulo smooth kernels. □

PROPOSITION 8.7.2. *Let $\omega_{2\mathbb{C}} \in \mathcal{D}'(V)$ a distribution as in Definition* 8.2.1. *Then*

$$\mathrm{WF}(\omega_{2\mathbb{C}})' \subset \mathcal{N}^+ \times \mathcal{N}^+. \tag{8.15}$$

The proof below shows that actually $\mathrm{WF}(\omega_{2\mathbb{C}})' \subset \mathcal{C}^+$, where $\mathcal{C}^+$ is defined in (7.22).

Proof. We first estimate the wavefront set of $(Q^{-1})_+$ and $(\log Q)_+$.

If $x_0\cdot\eta x_0 \neq 0$, then near x_0 we have $(Q^{-1})_+(x) = Q^{-1}(x)$ and $(\log Q)_+(x) = \log|Q(x)| + \mathrm{i}\theta$, where $\theta = 0$ if $x_0\cdot\eta x_0 > 0$, and $\theta = \pm\pi$ if $x_0 \in C_\pm$. In particular, $(Q^{-1})_+$ and $(\log Q)_+$ are smooth in $\{x\cdot\eta x \neq 0\}$.

If $x_0\cdot\eta x_0 = 0$ and $x_0 \neq 0$, then $Q(x_0 + \mathrm{i}y) = -y\cdot\eta y + 2\mathrm{i}x_0\cdot\eta y$. It follows that $Q^{-1}(x+\mathrm{i}y)$ and $\log Q(x+\mathrm{i}y)$ are holomorphic in $U_{x_0} + \mathrm{i}\Gamma_{x_0}$ where $U_{x_0} \subset \mathbb{R}^n$ is a small neighborhood of x_0 and $\Gamma_{x_0} = \{y \in \mathbb{R}^n : \pm x_0\cdot\eta y > 0\}$ for $x_0 \in N_\pm$.

Finally, we saw in Section 8.2 that $Q^{-1}(x+\mathrm{i}y)$ and $\log Q(x+\mathrm{i}y)$ are holomorphic in $U_0 + \mathrm{i}\Gamma_0$, where $U_0 \subset \mathbb{R}^n$ is a small neighborhood of 0 and $\Gamma_0 = C_+$, and that Q^{-1} and $\log Q$ are of moderate growth in $U_{x_0} + \mathrm{i}K$, where U_{x_0} is a small neighborhood of x_0 and $K \Subset \Gamma_{x_0}$ is any relatively compact cone. Note that the cone Γ_{x_0}always contains C_+.

From Section 12.2 we obtain the estimate

$$\mathrm{WF}((Q^{-1})_+), \mathrm{WF}((\log Q)_+) \subset \bigcup_{x_0\in N} x_0 \times \Gamma_{x_0}^\circ,$$

where the *polar cone* Γ° of a cone $\Gamma \subset \mathbb{R}^n$ is the set

$$\Gamma^\circ := \{\xi \in (\mathbb{R}^n)' \setminus o : x\cdot\xi \geq 0,\ \forall x \in \Gamma\}. \tag{8.16}$$

It follows that

$$\begin{aligned}&\mathrm{WF}((Q^{-1})_+), \mathrm{WF}((\log Q)_+)\\ &\subset \{(x, \pm\lambda\eta x) : x \in N_\pm, x \neq 0, \lambda > 0\} \cup \{(0,\xi) : \xi\cdot\eta^{-1}\xi = 0, \xi_0 > 0\},\end{aligned} \tag{8.17}$$

where $\xi_0 = \xi\cdot e^0$, $e^0 = (1,\dots,0)$.

Let now $u = (Q^{-1})_+$ or $(\log Q)_+ \in \mathcal{D}'(\mathbb{R}^n)$, and let $F : V \to \mathbb{R}^n$ be the map in (8.11). By Subsection 7.2.4, we have

$$\mathrm{WF}(F^*u)' \subset \{\big((x, {}^tD_xF\xi), (x', -{}^tD_{x'}F\xi)\big) : (F(x,x'),\xi) \in \mathrm{WF}u\}. \tag{8.18}$$

Note that we can forget the isometry $R(x')$ in the definition of F if we introduce the orthonormal frame $e^i(x) = R^{-1}(x)e^i$, where $(e^1,\dots,e^n)$ is the canonical basis of $\mathbb{R}^n$.

Let us first estimate $\mathrm{WF}(F^*u)'$ away from the diagonal $x = x'$. We obtain from (8.17) that the right-hand side in (8.18) is included in

$$\{\big((x, \lambda {}^tD_xF\eta v), (x', -\lambda {}^tD_{x'}F\eta v)\big) : v = F(x,x') \in N, \lambda v \in N_+\}.$$

Since $\sigma(x,x') = F(x,x')\cdot\eta F(x,x')$, we have

$$D_x\sigma(x,x') = 2D_xF(x,x')\cdot\eta F(x,x'),\ D_x\sigma(x,x') = 2D_{x'}F(x,x')\cdot\eta F(x,x'),$$

hence the set above equals

$$\{((x, \lambda D_x\sigma), (x', -\lambda D_{x'}\sigma)) : v = F(x,x') \in N, \lambda v \in N_+\}. \tag{8.19}$$

By the Gauss lemma, the radial geodesic between x' and x is normal to the hypersurface $\sigma(\cdot,x') = Cst$, which implies that the vectors $\lambda\nabla_x\sigma(x,x'), -\lambda\nabla_{x'}\sigma(x,x')$ are tangent to the (null) geodesic between x' and x, and future pointing. This

implies that the set in (8.19) is included in $\mathcal{N}^+ \times \mathcal{N}^+$ (actually in $\mathcal{C}^+$). Let us now estimate $\mathrm{WF}(F^*u)'$ above the diagonal $x = x'$. If we work in normal coordinates at x, we have $D_x F = \mathbb{1}$, $D_{x'} F = -\mathbb{1}$ at (x, x) hence above the diagonal we have also $\mathrm{WF}(F^*u)' \subset \{(X, X) : X \in \mathcal{N}^+\}$.

In conclusion we have shown that $\mathrm{WF}((\sigma^{-1})_+)'$ and $\mathrm{WF}((\log\sigma)_+)'$ are included in the right-hand side of (8.15). This implies the same estimate for $\mathrm{WF}(\omega_2)'$. □

8.8. Examples of Hadamard states

Let us consider one of the simplest examples of globally hyperbolic spacetimes, namely *ultra-static spacetimes*, see Section 5.3. We assume that (S, h) is complete. More examples will be given in Chapter 9.

The associated Klein-Gordon operator $P = -\Box_g + m^2$ for $m > 0$ is

$$\partial_t^2 + \epsilon^2,$$

where $\epsilon^2 = -\Delta_h + m^2$ is essentially selfadjoint on $C_0^\infty(S)$. By Subsection 4.10.3, we can construct the *vacuum state* ω_{vac} for P, whose spacetime covariances are given by the analog of (4.47):

$$(u|\Lambda^{\pm}_{\mathrm{vac}} v) = \int_{\mathbb{R}} (u(t,\cdot)|\frac{1}{2\epsilon}\mathrm{e}^{\pm \mathrm{i}t\epsilon} v(t,\cdot))_S dt, \quad u, v \in C_0^\infty(\mathbb{R}\times S),$$

where $(u|v)_S = \int_S \overline{u} v \, dVol_h$ and $u_t(\cdot) = u(t,\cdot)$.

One can similarly express the Feynman inverse associated to ω_{vac}, which equals

$$G_{\mathrm{F}} u(t,\cdot) = \int_{\mathbb{R}} G_{\mathrm{F}}(t-t') u(t',\cdot) dt',$$

with

$$G_{\mathrm{F}}(t) = (2\mathrm{i}\epsilon)^{-1}\left(\mathrm{e}^{\mathrm{i}t\epsilon}\theta(t) + \mathrm{e}^{-\mathrm{i}t\epsilon}\theta(-t)\right). \tag{8.20}$$

THEOREM 8.8.1. *The vacuum state ω_{vac} is a pure Hadamard state.*

Proof. We saw in Subsection 4.10.3 that ω_{vac} is a pure state. It suffices then to verify (genHad). Since $m > 0$, we see that $\Lambda^{\pm}_{\mathrm{vac}} : L^2(\mathbb{R}\times S) \to L^2(\mathbb{R}\times S)$ have distributional kernels. We have $\Lambda^{\pm}_{\mathrm{vac}}(t,t,\mathrm{x},\mathrm{x}') = F^{\pm}(t-t',\mathrm{x},\mathrm{x}')$ for $F^{\pm}u = (2\epsilon)^{-1}\mathrm{e}^{\pm \mathrm{i}t\epsilon}u$, $u \in C_0^\infty(S)$. By Subsection 7.2.4, it suffices to show that $\mathrm{WF}(F^{\pm})' \subset \{\pm\tau > 0\} \times T^*S \times T^*S$. But this follows from Proposition 7.1.5, since if we set $G^{\pm}(z)u = (2\epsilon)^{-1}\mathrm{e}^{\pm \mathrm{i}z\epsilon}u$, $u \in C_0^\infty(S)$, functional calculus shows that $G^{\pm}(z,\cdot)$ is holomorphic in $\{\pm\mathrm{Im}\, z > 0\}$ with values in $\mathcal{D}'(S\times S)$ with $F^{\pm}(t,\cdot) = G^{\pm}(t \pm \mathrm{i}0, \cdot)$. □

8.9. Existence of Hadamard states

In this subsection we prove the important result of Fulling, Narcowich and Wald [**FNW**], about *existence* of Hadamard states.

THEOREM 8.9.1. *Let P be a Klein-Gordon operator on a globally hyperbolic spacetime (M, g). Then there exists a* pure *Hadamard state for P.*

Proof. By Theorem 5.4.4 we can assume that $M = \mathbb{R}\times\Sigma$ and $g = -\beta(t,\mathrm{x})dt^2 + h_t(\mathrm{x})d\mathrm{x}^2$, where Σ is a Cauchy surface of (M, g). We fix an ultra-static metric $g_{\mathrm{us}} = -dt^2 + h(\mathrm{x})d\mathrm{x}^2$ and an interpolating metric $g_{\mathrm{int}} = \chi_-(t)g_{\mathrm{us}} + \chi_+(t)g$, with cutoff functions $\chi_\pm$ such that $g_{\mathrm{int}} = g_{\mathrm{us}}$ in $\{t \le -T+1\}$, $g_{\mathrm{int}} = g$ in $\{t \ge T-1\}$.

We set $P_{\mathrm{us}} = -\Box_{g_{\mathrm{us}}} + m^2$, $m > 0$, and fix a Klein-Gordon operator P_{int} for g_{int} such that $P_{\mathrm{int}} = P_{\mathrm{us}}$ in $\{t \le -T+1\}$, $P_{\mathrm{int}} = P$ in $\{t \ge T-1\}$.

For $\Sigma_{\pm T} = \{\pm T\} \times \Sigma$, we denote by $\lambda^{\pm}_{-T,\mathrm{vac}}$ the Cauchy surface covariances on Σ_{-T} of the vacuum state ω_{us} for P_{us}. By Proposition 6.1.5, $\lambda^{\pm}_{-T,\mathrm{vac}}$ are also the Cauchy surface covariances of a *pure* state ω_{int} for P_{int}.

Since $P_{\mathrm{us}} = P_{\mathrm{int}}$ on a causally compatible neighborhood V of Σ_{-T}, we have $G_{\mathrm{vac}} = G_{\mathrm{int}}$ on $V \times V$. Therefore, the spacetime covariances of ω_{int} and ω_{us}, given in Proposition 6.1.6, coincide on $V \times V$. Since ω_{us} is a Hadamard state, the spacetime covariances $\Lambda^{\pm}_{\mathrm{int}}$ of ω_{int} satisfy (Had) over $V \times V$, hence everywhere by propagation of singularities, see e.g. (7.25).

Let now $\lambda^{\pm}_{T,\mathrm{int}}$ be the Cauchy surface covariances of ω_{int} on Σ_T. Again by Proposition 6.1.5, they are the Cauchy surface covariances of a pure state ω for P. By the same argument as above ω is a Hadamard state. □

CHAPTER 9

Vacuum and thermal states on stationary spacetimes

In this chapter we introduce the notions of *vacuum* and *thermal states* for Klein-Gordon fields on stationary spacetimes, see [**Ky1**], [**S2**]. These states are important examples of Hadamard states, the vacuum state giving in particular a preferred pure Hadamard state on a stationary spacetime.

9.1. Ground states and KMS states

It is convenient to introduce these notions first in an abstract framework. We work in the complex framework (to which the real one can be reduced).

Thus, let $(\mathcal{Y}, q)$ be a Hermitian space and $\{r_s\}_{s\in\mathbb{R}}$ be a unitary group on $(\mathcal{Y}, q)$, i.e. such that $r_s^* q r_s = q$ for $s \in \mathbb{R}$. It follows that $\{r_s\}_{s\in\mathbb{R}}$ induces a group $\{\tau_s\}_{s\in\mathbb{R}}$ of $*$-automorphisms of $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$ defined by $\tau_s(\psi^{(*)}(y)) = \psi^{(*)}(r_s y)$.

We recall the definitions, see e.g. [**S2**, Definitions 2.3, 2.4], of ground states and KMS states for $\{\tau_s\}_{s\in\mathbb{R}}$. We set $D_\beta = \mathbb{R}+\mathrm{i}]0,\beta[$ for $\beta > 0$, $D_\infty = \mathbb{R}+\mathrm{i}]0,+\infty[$.

Let ω be a state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$ which is *invariant* under $\{\tau_s\}_{s\in\mathbb{R}}$ i.e. $\omega(A) = \omega(\tau_s(A))$ for $s \in \mathbb{R}, A \in \mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q)$. Assume moreover that the function

$$\mathbb{R} \ni s \longmapsto \omega(A^* \tau_s B) \in \mathbb{C} \text{ is continuous for all } A, B \in \mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}, q). \tag{9.1}$$

It follows that if $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is the GNS triple for ω, see Subsection 4.4.1, there exists a selfadjoint operator H on $\mathcal{H}_\omega$ such that

$$\pi_\omega(\tau_s(A)) = \mathrm{e}^{\mathrm{i}sH} \pi_\omega(A) \mathrm{e}^{-\mathrm{i}sH}, \quad H\Omega_\omega = 0.$$

Definition 9.1.1. *A state ω is a* non-degenerate ground state *for $\{r_s\}_{s\in\mathbb{R}}$ if ω is invariant under $\{\tau_s\}_{s\in\mathbb{R}}$,* (9.1) *holds, and moreover*

$$H \geq 0, \quad \mathrm{Ker}\, H = \mathbb{C}\Omega_\omega. \tag{9.2}$$

Let us assume in addition that ω is gauge-invariant and quasi-free and let $\lambda^\pm$ be its complex covariances. Since $\omega(\psi^{(*)}(y)) = 0$, we know that $\pi_\omega(\psi^{(*)}(y))\Omega_\omega$ is orthogonal to Ω_ω.

It follows then from (9.2) and the spectral theorem that for all $y_1, y_2 \in \mathcal{Y}$ there exists a function $F^\pm_{y_1,y_2}$ holomorphic in D_∞, bounded and continuous in $\overline{D}_\infty$, such that

$$\begin{aligned} &F^+_{y_1,y_2}(s) = \overline{y}_1 \cdot \lambda^+ r_s y_2, \quad F^-_{y_1,y_2}(s) = \overline{r_s y}_1 \cdot \lambda^+ y_2, \\ &\lim_{\sigma\to+\infty} \sup_{s\in\mathbb{R}} |F^\pm_{y_1,y_2}(s + \mathrm{i}\sigma)| = 0. \end{aligned} \tag{9.3}$$

Definition 9.1.2. *A state ω is a* KMS state *at temperature $T = \beta^{-1}$ if for all $A_1, A_2 \in \mathrm{CCR}(\mathcal{Y}, q)$ there exists a function F_{A_1,A_2} holomorphic in D_β, bounded and continuous in $\overline{D}_\beta$, such that*

$$\begin{aligned} &F_{A_1,A_2}(s) = \omega(A_1 \tau_s(A_2)), \\ &F_{A_1,A_2}(s + \mathrm{i}\beta) = \omega(\tau_s(A_2) A_1), \quad s \in \mathbb{R}. \end{aligned}$$

If ω is gauge-invariant and quasi-free, taking $A_1 = \psi(y_1)$, $A_2 = \psi^*(y_2)$, we obtain as above that for all $y_1, y_2 \in \mathcal{Y}$ there exists a function F_{y_1,y_2} holomorphic in D_β, bounded and continuous in $\overline{D}_\beta$, such that

$$F_{y_1,y_2}(s) = \overline{y}_1 \cdot \lambda^+ r_s y_2, \quad F_{y_1,y_2}(s + \mathrm{i}\beta) = \overline{y}_1 \cdot \lambda^- r_s y_2. \tag{9.4}$$

9.1.1. Positivity of the energy. We now prove an important result, due to Kay and Wald [**KW**, Section 6.2], which relates the existence of ground or KMS states to the positivity of the classical energy associated to $\{r_s\}_{s\in\mathbb{R}}$.

THEOREM 9.1.3. *Let $(\mathcal{Y}, q, \{r_s\}_{s\in\mathbb{R}})$ be as above and ω be a quasi-free non-degenerate ground state or a quasi-free* KMS *state. Assume moreover that $\mathcal{Y}$ is equipped with a vector space topology for which $\lambda^\pm, q$ are continuous and such that $\partial_s r_s y = \mathrm{i} b r_s y$, for all $y \in \mathcal{Y}$ for some $b \in L(\mathcal{Y})$. Then the* classical energy *associated to $\{r_s\}_{s\in\mathbb{R}}$ $E = qb$ is positive.*

Proof. Since $q = \lambda^+ - \lambda^-$ is non-degenerate, $(\cdot|\cdot)_\omega = \lambda^+ + \lambda^-$ is a Hilbertian scalar product on $\mathcal{Y}$ and we denote by $\mathcal{Y}^{\mathrm{cpl}}$ the completion of $\mathcal{Y}$ with respect to $(\cdot|\cdot)_\omega$. We still denote by $\lambda^\pm, q$ the bounded extensions of $\lambda^\pm, q$ to $\mathcal{Y}^{\mathrm{cpl}}$.

The state ω is τ_s invariant, which implies that $r_s^* \lambda^\pm r_s = \lambda^\pm$. Moreover by Definitions 9.1.1 and 9.1.2, the map $\mathbb{R} \ni s \mapsto \overline{y}_1 \cdot \lambda^\pm r_s y_2 \in \mathbb{C}$ is continuous for $y_1, y_2 \in \mathcal{Y}$. It follows that $\{r_s\}_{s\in\mathbb{R}}$ extends to a weakly, hence strongly continuous unitary group $\{\mathrm{e}^{\mathrm{i}sb^{\mathrm{cpl}}}\}_{s\in\mathbb{R}}$ on $\mathcal{Y}^{\mathrm{cpl}}$, with b^{cpl} selfadjoint on $\mathcal{Y}^{\mathrm{cpl}}$. We have $b^{\mathrm{cpl}}|_{\mathcal{Y}} = b$ and $\mathcal{Y}$ is a core for b^{cpl} by Nelson's invariant domain theorem.

We first check that (9.3), (9.4) extend to $y_i \in \mathcal{Y}^{\mathrm{cpl}}$ with r_s replaced by $\mathrm{e}^{\mathrm{i}sb^{\mathrm{cpl}}}$. Let $y_1, y_2 \in \mathcal{Y}^{\mathrm{cpl}}$, $y_{i,n} \in \mathcal{Y}$ with $y_{i,n} \to y_i$ in $\mathcal{Y}^{\mathrm{cpl}}$, and let $F_n = F_{y_{1,n},y_{2,n}}$. Note that $F_n(t) \to \overline{y}_1 \cdot \lambda^+ \mathrm{e}^{\mathrm{i}tb^{\mathrm{cpl}}} y_2$ and $F_n(t + \mathrm{i}\beta) \to \overline{y}_1 \cdot \lambda^- \mathrm{e}^{\mathrm{i}tb^{\mathrm{cpl}}} y_2$ uniformly on $\mathbb{R}$. It follows from the three lines theorem that

$$\sup_{z\in D_\beta} |F_n(z) - F_m(z)| \leq \sup_{s\in\mathbb{R}\cup\mathbb{R}+\mathrm{i}\beta} |F_n(s) - F_m(s)|, \quad \beta < \infty$$
$$\sup_{z\in D_\infty} |F_n(z) - F_m(z)| \leq \sup_{s\in\mathbb{R}} |F_n(s) - F_m(s)|.$$

Therefore, F_n converges uniformly in $\overline{D}_\beta$ to F_{y_1,y_2}, which is holomorphic in D_β, bounded and continuous in $\overline{D}_\beta$ for $\beta \in]0, +\infty]$ and satisfies (9.3), resp. (9.4).

Let us first assume that $\beta < \infty$. If we choose $y_1, y_2 \in \mathcal{Y}^{\mathrm{cpl}}$ with y_2 an entire vector for b^{cpl}, we have $F_{y_1,y_2}(z) = \overline{y}_1 \cdot \lambda^+ \mathrm{e}^{\mathrm{i}zb^{\mathrm{cpl}}} y_2$, which using (9.4) implies that

$$\overline{y}_1 \cdot \lambda^+ \mathrm{e}^{-\beta b^{\mathrm{cpl}}} y_2 = \overline{y}_1 \cdot \lambda^- y_2,$$

and hence, using that $\lambda^+ - \lambda^- = q$,

$$\lambda^+ (1 - \mathrm{e}^{-\beta b^{\mathrm{cpl}}}) = \lambda^- (\mathrm{e}^{\beta b^{\mathrm{cpl}}} - 1) = q.$$

This implies that $(\lambda^+ + \lambda^-) \tanh(\beta b^{\mathrm{cpl}}/2) = q$. Let us set $B = b^{\mathrm{cpl}} \tanh(\beta b^{\mathrm{cpl}}/2)$. By functional calculus $\mathrm{Dom}\, B = \mathrm{Dom}\, b^{\mathrm{cpl}}$. If $y \in \mathcal{Y} \subset \mathrm{Dom}\, B$, we have

$$(y|By)_\omega = \overline{y} \cdot (\lambda^+ + \lambda^-) By = \overline{y} \cdot q b^{\mathrm{cpl}} y = \overline{y} \cdot qby = \overline{y} \cdot Ey,$$

where $E = qb$ is the classical energy associated to $\{r_s\}_{s\in\mathbb{R}}$. Since $B \geq 0$ for $(\cdot|\cdot)_\omega$ this proves the proposition for $\beta < \infty$.

Now assume that $\beta = \infty$. For y an entire vector for b^{cpl}, we have

$$F^+_{y,y}(z) = \overline{y} \cdot \lambda^+ \mathrm{e}^{\mathrm{i}zb^{\mathrm{cpl}}} y, \quad F^-_{y,y}(z) = \overline{\mathrm{e}^{\mathrm{i}\overline{z}b^{\mathrm{cpl}}} y} \cdot \lambda^- y.$$

Let $A^\pm \in B(\mathcal{Y}^{\mathrm{cpl}})$ be such that $\overline{y}_1 \cdot \lambda^\pm y_2 = (y_1|A^\pm y_2)_\omega$. We have $A^\pm \geq 0$ and $[A^\pm, \mathrm{e}^{\mathrm{i}sb^{\mathrm{cpl}}}] = 0$ by the invariance of ω under τ_s. From (9.3) we obtain that

$$\lim_{\sigma\to+\infty} (y|A^+ \mathrm{e}^{-\sigma b^{\mathrm{cpl}}} y)_\omega = \lim_{\sigma\to+\infty} (y|\mathrm{e}^{\sigma b^{\mathrm{cpl}}} A^- y)_\omega = 0,$$

i.e. $\lim_{\sigma\to+\infty}\|\mathrm{e}^{\mp\sigma b^{\mathrm{cpl}}/2}(A^{\pm})^{\frac{1}{2}}y\|=0$. This implies that

$$\mathbb{1}_{\mathbb{R}^-}(b^{\mathrm{cpl}})(A^+)^{\frac{1}{2}}y=\mathbb{1}_{\mathbb{R}^+}(b^{\mathrm{cpl}})(A^-)^{\frac{1}{2}}y=0,\quad \mathbb{R}^{\pm}=\pm[0,+\infty[\,,$$

hence $\lambda^{\pm}\mathbb{1}_{\mathbb{R}^{\pm}}(b^{\mathrm{cpl}})=0$ by density. For $y\in\mathcal{Y}$ we then have

$$\overline{y}\cdot qby=\overline{y}\cdot\lambda^+by-\overline{y}\cdot\lambda^-by=\overline{y}\cdot\lambda^+\mathbb{1}_{\mathbb{R}^+}(b^{\mathrm{cpl}})b^{\mathrm{cpl}}y-\overline{y}\cdot\lambda^-\mathbb{1}_{\mathbb{R}^-}(b^{\mathrm{cpl}})b^{\mathrm{cpl}}y$$

$$=\quad (y|(A^++A^-)|b^{\mathrm{cpl}}|y)_\omega=(y||b^{\mathrm{cpl}}|^{\frac{1}{2}}(A^++A^-)|b^{\mathrm{cpl}}|^{\frac{1}{2}}y)_\omega\geq 0,$$

which completes the proof if $\beta=\infty$. □

9.1.2. Existence of ground and KMS states. We saw in Theorem 9.1.3 that the positivity of the classical energy is a necessary condition for the existence of a ground or KMS state. Let us now describe the converse result.

Let $(\mathcal{Y},q)$ be a Hermitian space and $E\in L_{\mathrm{h}}(\mathcal{Y},\mathcal{Y}^*)$ with $E>0$, the function $\mathcal{Y}\ni y\mapsto\overline{y}\cdot Ey$ being the classical energy. The *energy space* $\mathcal{Y}_{\mathrm{en}}$ is the completion of $\mathcal{Y}$ for the scalar product $(y_1|y_2)_{\mathrm{en}}=\overline{y}_1\cdot Ey_2$ and is a complex Hilbert space. Let $r_s=\mathrm{e}^{\mathrm{i}sb}$ be a strongly continuous unitary group on $\mathcal{Y}_{\mathrm{en}}$ with selfadjoint generator b. We assume that $r_s:\mathcal{Y}\to\mathcal{Y}$, $\mathcal{Y}\subset\operatorname{Dom}b$, $\operatorname{Ker}b=\{0\}$, and

$$\overline{y}_1\cdot Ey_2=\overline{y}_1\cdot qby_2,\quad y_1,y_2\in\mathcal{Y}. \tag{9.5}$$

The meaning of (9.5) is that $\{r_s\}_{s\in\mathbb{R}}$ is the symplectic evolution group associated to the classical energy $\overline{y}\cdot Ey$ and the symplectic form $\sigma=\mathrm{i}^{-1}q$.

One introduces then the *dynamical Hilbert space*

$$\mathcal{Y}_{\mathrm{dyn}}:=|b|^{\frac{1}{2}}\mathcal{Y}_{\mathrm{en}},$$

see [**DG**, Subsection 18.2.1], with the scalar product $(y_1|y_2)_{\mathrm{dyn}}=(y_1||b|^{-1}y_2)_{\mathrm{en}}$. The group $\{r_s\}_{s\in\mathbb{R}}$ extends obviously as a unitary group on $\mathcal{Y}_{\mathrm{dyn}}$ whose generator will be still denoted by b.

From (9.5) we obtain that

$$\overline{y}_1\cdot qy_2=(y_1|\mathrm{sgn}(b)y_2)_{\mathcal{Y}_{\mathrm{dyn}}} \tag{9.6}$$

so q is a bounded sesquilinear form on $\mathcal{Y}_{\mathrm{dyn}}$, but in general not on $\mathcal{Y}_{\mathrm{en}}$, unless $0\notin\sigma(b)$.

Definition 9.1.4. *The* ground state ω_∞ *is defined by the covariances*

$$\overline{y}_1\cdot\lambda^{\pm}_\infty y_2=(y_1|\mathbb{1}_{\mathbb{R}^{\pm}}(b)y_2)_{\mathrm{dyn}}. \tag{9.7}$$

Definition 9.1.5. *The* β-KMS state ω_β *is defined by the covariances*

$$\begin{aligned}\overline{y}_1\cdot\lambda^+_\beta y_2&=\overline{y}_1\cdot q(1-\mathrm{e}^{-\beta b})^{-1}y_2,\\ \overline{y}_1\cdot\lambda^-_\beta y_2&=\overline{y}_1\cdot q(\mathrm{e}^{\beta b}-1)^{-1}y_2.\end{aligned} \tag{9.8}$$

9.1.3. Infrared problem. The covariances $\lambda^{\pm}_\infty$ and $\lambda^{\pm}_\beta$ are a priori not defined on $\mathcal{Y}$ if $0\in\sigma(b)$. This is usually called an *infrared problem*.

However, if

$$\mathcal{Y}\subset\mathcal{Y}_{\mathrm{dyn}}\cap|b|^{\frac{1}{2}}\mathcal{Y}_{\mathrm{dyn}} \tag{9.9}$$

then using that $(1-\mathrm{e}^{\lambda})^{-1}$ behaves like λ^{-1} near $\lambda=0$, we see that $\lambda^{\pm}_\infty$ and $\lambda^{\pm}_\beta$ are well defined on $\mathcal{Y}$, and hence ω_∞ and ω_β are well defined quasi-free states on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},q)$.

Note that (9.9) is equivalent to

$$\overline{y}\cdot E|b|^{-1}y<\infty,\quad \overline{y}\cdot Eb^{-2}y<\infty,\ \ \forall y\in\mathcal{Y},$$

which follows from

$$\overline{y}\cdot Eb^{-2}y<\infty,\ \ \forall y\in\mathcal{Y}, \tag{9.10}$$

since $\mathcal{Y} \subset \mathcal{Y}_{\rm en}$.

9.1.4. Pure invariant states. Let $(\mathcal{Y}, q)$ be a Hermitian space with a unitary group $\{r_s\}_{s\in\mathbb{R}}$. Assume that $r_s = \mathrm{e}^{\mathrm{i}sb}$ on $\mathcal{Y}$ and that the classical energy $E = qb$ is positive definite on $\mathcal{Y}$. Then any pure state invariant under the induced group $\{\tau_s\}_{s\in\mathbb{R}}$ is actually equal to the ground state ω_∞.

As in Theorem 9.1.3, by $r_s = \mathrm{e}^{\mathrm{i}sb}$ on $\mathcal{Y}$ we mean that $\mathcal{Y}$ is equipped with a vector space topology for which q is continuous and such that $\partial_s r_s y = \mathrm{i}br_s y$, for all $y \in \mathcal{Y}$ for some $b \in L(\mathcal{Y})$. The classical energy $E = qb \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$ is thus well defined.

PROPOSITION 9.1.6. *Let ω a quasi-free state on $\mathrm{CCR}(\mathcal{Y}, q)$ such that its covariances $\lambda^\pm$ are continuous in the topology of $\mathcal{Y}$. Assume that ω is pure and invariant under the induced group $\{\tau_s\}_{s\in\mathbb{R}}$, and that E is positive definite on $\mathcal{Y}$. Then $\omega = \omega_\infty$.*

Proof. As in the proof of Theorem 9.1.3, we obtain that $\{r_s\}_{s\in\mathbb{R}}$ extends as a strongly continuous unitary group on the completion $\mathcal{Y}^{\rm cpl}$ of $\mathcal{Y}$ for $(\cdot|\cdot)_\omega$, whose generator $b^{\rm cpl}$ has $\mathcal{Y}$ as a core.

Since ω is pure, we deduce from Proposition 4.9.3 that there exist projections $c^\pm \in B(\mathcal{Y}^{\rm cpl})$, selfadjoint for $(\cdot|\cdot)_\omega$, with $c^+ + c^- = \mathbb{1}$, $\lambda^\pm = \pm qc^\pm$. From the invariance of ω we see that $[c^\pm, b^{\rm cpl}] = 0$. Next we compute for $y \in \mathcal{Y}$:

$$(y|(c^+ - c^-)b^{\rm cpl}y)_\omega = \overline{y}\cdot qby = \overline{y}\cdot Ey.$$

Since $\mathcal{Y}$ is a core for $b^{\rm cpl}$, this implies, by the uniqueness of the polar decomposition of $b^{\rm cpl}$, that $c^+ - c^- = \mathrm{sgn}(b^{\rm cpl})$, i.e. $c^\pm = \mathbb{1}_{\mathbb{R}^\pm}(b^{\rm cpl})$.

From this fact we deduce that $\mathcal{Y}^{\rm cpl}$ is the dynamical Hilbert space $\mathcal{Y}^{\rm dyn}$ introduced in 9.1.2, and hence $\omega = \omega_\infty$. □

9.2. Klein-Gordon operators

Let us now go back to a concrete situation and consider a globally hyperbolic spacetime (M, g) with a complete Killing vector field X. For the moment we do not assume X to be time-like. Assume that there exists a space-like Cauchy surface Σ transverse to X. If n is the future directed normal vector field to Σ, we have

$$X = Nn + w \quad \text{on } \Sigma, \tag{9.11}$$

where $N \in C^\infty(\Sigma; \mathbb{R})$ is called the *lapse function* and w^i is a smooth vector field on Σ called the *shift vector field*.

We can identify M with $\mathbb{R}_t \times \Sigma_y$ by the map

$$\chi : \mathbb{R} \times \Sigma \ni (t, y) \longmapsto \psi_t(y) \in M,$$

where ψ_t is the flow of X. We have

$$\chi^* g = -N^2(y)dt^2 + h_{ij}(y)(dy^i + w^i(y)dt)(dy^j + w^j(y)dy^j), \quad \chi^* X = \frac{\partial}{\partial t}. \tag{9.12}$$

It follows that X is time-like at y iff

$$N^2(y) > w^i(y)h_{ij}(y)w^j(y), \tag{9.13}$$

and space-like at y iff

$$N^2(y) < w^i(y)h_{ij}(y)w^j(y), \tag{9.14}$$

where h is the induced metric on Σ.

We fix a Klein-Gordon operator on (M, g) of the form

$$P = -\Box_g + V, \quad V \in C^\infty(M; \mathbb{R}) \text{ with } X\cdot V = 0. \tag{9.15}$$

The flow $\{\psi_s\}_{s\in\mathbb{R}}$ of X induces then a unitary group $\{r_s\}_{s\in\mathbb{R}}$ on the Hermitian spaces $(\frac{C_0^\infty(M)}{PC_0^\infty(M)}, (\cdot\,|\mathrm{i}G\,\cdot)_M)$, $(\mathrm{Sol}_{\mathrm{sc}}(P), q)$, defined as:

$$r_s[u] = [u\circ\psi_s],\ u\in C_0^\infty(M),\quad r_s\phi = \phi\circ\psi_s,\ \phi\in\mathrm{Sol}_{\mathrm{sc}}(P).$$

9.2.1. A non-existence result. The next proposition, due to Kay and Wald [**KW**, Subsection 6.2], shows that the fact that X is everywhere time-like on Σ, i.e. that (M,g) is stationary, is a necessary condition for the existence of a ground or KMS state for X.

PROPOSITION 9.2.1. *Let (M,g) a globally hyperbolic spacetime with a complete Killing vector field X and let $P=-\Box_g+V$, where $V\in C^\infty(M;\mathbb{R})$ with $X\cdot V=0$. Let $\{\tau_s\}_{s\in\mathbb{R}}$ be the group of $*$-automorphisms of* CCR(P) *induced by X.*

Assume that there exists a Cauchy surface Σ such that X is transverse to Σ and space-like *at some $y_0\in\Sigma$. Then there exists no* KMS *state nor non-degenerate ground state on* CCR(P) *for $\{\tau_s\}_{s\in\mathbb{R}}$.*

Proof. We identify M with $\mathbb{R}\times\Sigma$, the metric g being then as in (9.12). We choose $(\mathcal{Y},q)=(\mathrm{Sol}_{\mathrm{sc}}(P),q)$ with q defined in (5.35) and $r_s\phi(t,y)=\phi(t+s,y)$.

We identify $(\mathrm{Sol}_{\mathrm{sc}}(P),q)$ with $(C_0^\infty(\Sigma);\mathbb{C}^2,q_\Sigma)$ for q_Σ defined in (5.31) using ϱ_Σ and denote still by $\{r_s\}_{s\in\mathbb{R}}$ the image of r_s on $(C_0^\infty(\Sigma);\mathbb{C}^2,q_\Sigma)$. A standard computation shows that for $f\in C_0^\infty(\Sigma;\mathbb{C}^2)$, $\partial_s r_s f=\mathrm{i}NHr_sf$, where H is defined in (9.20). The associated energy $E=qH$ is given by (9.21) below.

For $y_0\in\Sigma$ we introduce local coordinates on Σ near y_0, fix $\chi\in C_0^\infty(U)$ for U a small neighborhood of y_0 in Σ, and set $f_0^\lambda(y)=\mathrm{e}^{\mathrm{i}\lambda\eta_0\cdot y}\chi(y)$, $f_1^\lambda=\mathrm{i}N^{-1}wf_0^\lambda$ for $\lambda\gg1$ and $\eta_0\in T^*_{y_0}\Sigma$. Then we have

$$\overline{f^\lambda}\cdot Ef^\lambda=\lambda^2\int_\Sigma\chi^2(y)(\eta_0\cdot h^{-1}(y)\eta_0-N^{-2}(y)(\eta_0\cdot w(y))^2)|h|^{\frac12}dy+O(\lambda). \tag{9.16}$$

If $X=\frac{\partial}{\partial t}$ is space-like at y_0, then $N^2(y_0)<w^i(y_0)h_{ij}(y_0)w^j(y_0)$, and so there exists a neighborhood U of y_0 in Σ such that

$$\eta_0\cdot h^{-1}(y)\eta_0-N^{-2}(y)(\eta_0\cdot w(y))^2<0,\quad y\in U,\ \text{for } \eta_0=h(y_0)w(y_0).$$

By (9.16) we obtain that $\overline{f^\lambda}\cdot Ef^\lambda<0$ for $\lambda\gg1$. This is a contradiction by Theorem 9.1.3. □

9.3. The Klein-Gordon equation on stationary spacetimes

We assume now that the Killing vector field is everywhere time-like and consider a Klein-Gordon operator $P=-\Box_g+V$. We will assume that V is preserved by the Killing field X and is *strictly positive*:

$$X\cdot V=0,\quad V>0.$$

REMARK 9.3.1. *Of course, the condition $X\cdot V=0$ is necessary for P to be invariant under the flow of X. The condition $V>0$ is used in Section 9.5to ensure that the covariances of the vacuum and thermal state are well defined on $C_0^\infty(\Sigma;\mathbb{C}^2)$, i.e. to avoid a possible infrared problem. If V takes large negative values the conserved energy E defined in* (9.21) *may not be positive. In this case it seems impossible to construct vacuum or* KMS *states.*

The Klein-Gordon operator P takes the form

$$P=(\partial_t+w^*)N^2(\partial_t+w)+h_0, \tag{9.17}$$

with

$$h_0=\nabla^*h^{-1}\nabla+V,\ w=w^i\partial_{y^i}, \tag{9.18}$$

where in (9.17) and (9.18) the adjoints are computed with respect to the scalar product

$$(u|v) = \int_{\mathbb{R}\times\Sigma} \overline{u} v N|h|^{\frac{1}{2}} dtdy.$$

We denote by $\tilde{\mathcal{H}}$ the Hilbert space $L^2(\Sigma, N|h|^{\frac{1}{2}}dy)$. Let us point out a useful operator inequality which follows from (9.13).

LEMMA 9.3.2. *One has*

$$h_0 \geq w^* N^{-2} w + V \text{ on } C_0^\infty(\Sigma), \quad \text{for the scalar product of } \tilde{\mathcal{H}}.$$

Proof. Let $\mathcal{X}$ be a real vector space, $k \in L_{\rm s}(\mathcal{X}, \mathcal{X}')$ be strictly positive, and $c \in \mathcal{X}$. Then for $\gamma = kc \in \mathcal{X}'$ and $\xi \in \mathbb{C}\mathcal{X}'$ we have

$$\begin{aligned} & (\overline{\xi} - \langle\overline{\xi}|c\rangle\gamma)\cdot k^{-1}(\xi - \langle\xi|c\rangle\gamma) \\ = \;& \overline{\xi}\cdot k^{-1}\xi - 2\mathrm{Re}(\langle\overline{\xi}|c\rangle\gamma\cdot k^{-1}\xi) + |\langle\xi|c\rangle|^2\gamma\cdot k^{-1}\gamma \\ = \;& \overline{\xi}\cdot k^{-1}\xi - (2 - c\cdot kc)|\langle\xi|c\rangle|^2, \end{aligned}$$

whence

$$k^{-1} - |c\rangle\langle c| \geq (1 - c\cdot kc)|c\rangle\langle c|. \tag{9.19}$$

For $u \in C_0^\infty(\Sigma)$ we write

$$(u|(h_0 - w^* N^{-2} w)u) = \int_\Sigma \left[(\partial_{y^i}\overline{u}(h^{ij} - w^i N^{-2} w^j)\partial_{y^j} u + V|u|^2\right] N|h|^{\frac{1}{2}} dy.$$

Applying (9.19) under the integral sign for $k = h(y)$ and $c = N^{-1}(y)w^i(y)$, we obtain the lemma. □

If $\varrho_t : \mathrm{Sol}_{\rm sc}(P) \to C_0^\infty(\Sigma; \mathbb{C}^2)$ is the Cauchy data map on $\Sigma_t = \{t\}\times\Sigma$ we have, by (9.11) that

$$\varrho_t\phi = \begin{pmatrix} \phi(t,\cdot) \\ \mathrm{i}^{-1}N^{-1}(\partial_t - w)\phi(t,\cdot) \end{pmatrix},$$

and if we identify $\mathrm{Sol}_{\rm sc}(P)$ with $C_0^\infty(\Sigma; \mathbb{C}^2)$ using the map ϱ_0, we obtain that $r_s : C_0^\infty(\Sigma; \mathbb{C}^2) \to C_0^\infty(\Sigma; \mathbb{C}^2)$ is given by

$$r_s f = \varrho_s U_0 f, \; f \in C_0^\infty(\Sigma; \mathbb{C}^2),$$

where $\phi = U_0 f$ is the solution of the Cauchy problem

$$\begin{cases} P\phi = 0, \\ \varrho_0\phi = f. \end{cases}$$

An easy computation shows that:

$$N^{-1}\partial_s r_s f = \mathrm{i}H r_s f, H = \begin{pmatrix} -\mathrm{i}N^{-1}w & \mathbb{1} \\ h_0 & \mathrm{i}w^* N^{-1} \end{pmatrix}, \quad f \in C_0^\infty(\Sigma; \mathbb{C}^2). \tag{9.20}$$

The *classical energy*

$$\overline{f}\cdot \mathrm{E}f = \|f_1 - \mathrm{i}N^{-1}wf_0\|^2_{\tilde{\mathcal{H}}} + (f_0|h_0 f_0)_{\tilde{\mathcal{H}}} - (wf_0|N^{-2}wf_0)_{\tilde{\mathcal{H}}}, \tag{9.21}$$

and the *charge*

$$\overline{f}\cdot qf = (f_1|N^{-1}f_0)_{\tilde{\mathcal{H}}} + (f_0|N^{-1}f_1)_{\tilde{\mathcal{H}}}, \tag{9.22}$$

are both conserved by the evolution $\mathrm{e}^{\mathrm{i}sH}$ on $C_0^\infty(\Sigma; \mathbb{C}^2)$.

9.4. Reduction

It is useful to reduce (9.20) to a simpler evolution equation. To this end one introduces

$$\tilde{P} = NPN = (\partial_t + \tilde{w}^*)(\partial_t - \tilde{w}) + \tilde{h}_0,$$

for

$$\tilde{h}_0 = Nh_0N, \quad \tilde{w} = N^{-1}wN, \quad \tilde{w}^* = Nw^*N^{-1}. \tag{9.23}$$

Setting

$$\tilde{\varrho}_t\tilde{\phi} = \begin{pmatrix} \tilde{\phi}(t,\cdot) \\ \mathrm{i}^{-1}(\partial_t - \tilde{w})\tilde{\phi}(t,\cdot) \end{pmatrix}, \quad \tilde{H} = \begin{pmatrix} -\mathrm{i}\tilde{w} & \mathbb{1} \\ \tilde{h}_0 & \mathrm{i}\tilde{w}^* \end{pmatrix}, \tag{9.24}$$

we have

$$\begin{aligned} &\varrho_t N = Z\tilde{\varrho}_t \text{ on } C^\infty(M), \\ &N^{-1}\partial_s - \mathrm{i}H = Z'(\partial_s - \mathrm{i}\tilde{H})Z^{-1} \quad \text{on } C_0^\infty(\Sigma;\mathbb{C}^2), \end{aligned} \tag{9.25}$$

where

$$Z =: \begin{pmatrix} N & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \; Z' := \begin{pmatrix} \mathbb{1} & 0 \\ 0 & N^{-1} \end{pmatrix}, \tag{9.26}$$

Setting

$$\begin{aligned} &\overline{f}\cdot\tilde{E}f = \|f_1 - \mathrm{i}\tilde{w}f_0\|^2_{\tilde{\mathcal{H}}} + (f_0|\tilde{h}_0 f_0)_{\tilde{\mathcal{H}}} - (\tilde{w}f_0|\tilde{w}f_0)_{\mathcal{H}}, \\ &\overline{f}\cdot\tilde{q}f = (f_1|f_0)_{\tilde{\mathcal{H}}} + (f_0|f_1)_{\tilde{\mathcal{H}}}, \end{aligned}$$

we have

$$Z^*EZ = \tilde{E}, \quad Z^*qZ = \tilde{q} \text{ on } C_0^\infty(\Sigma;\mathbb{C}^2). \tag{9.27}$$

9.5. Ground and KMS states for P

From Lemma 9.3.2 we obtain that

$$\tilde{h}_0 - \tilde{w}^*\tilde{w} \geq VN^2, \tag{9.28}$$

which using that $V > 0$ implies that $\tilde{E} > 0$ on $C_0^\infty(\Sigma;\mathbb{C}^2)$. We can apply the abstract constructions in Subsection 9.1.2 provided we check (9.10). To check this condition we note that $bg = f$ is equivalent to

$$(\tilde{h}_0 - \tilde{w}^*\tilde{w})g_0 = f_1 - \mathrm{i}\tilde{w}^*f_0, \quad g_1 - \mathrm{i}\tilde{w}g_0 = f_0.$$

By Lemma 9.3.2, $\tilde{h}_0 - \tilde{w}^*\tilde{w} \geq NVN$ on $C_0^\infty(\Sigma)$. Let $\tilde{h}$ be the Friedrichs extension of $\tilde{h}_0 - \tilde{w}^*\tilde{w}$, acting on the Hilbert space $\tilde{\mathcal{H}}$. By the Kato-Heinz theorem, we have $\tilde{h}^{-1} \leq (NVN)^{-1}$, hence $C_0^\infty(\Sigma) \subset \mathrm{Dom}(NVN)^{-\frac{1}{2}} \subset \mathrm{Dom}\,\tilde{h}^{-\frac{1}{2}}$.

For $f \in C_0^\infty(\Sigma;\mathbb{C}^2)$, we can express $g = b^{-1}f$ as

$$g_0 = \tilde{h}^{-1}(f_1 - \mathrm{i}\tilde{w}^*f_0), \quad g_1 = g_0 + \mathrm{i}\tilde{w}\tilde{h}^{-1}(f_1 - \mathrm{i}\tilde{w}^*f_0),$$

noting that $f_1 - \mathrm{i}\tilde{w}^*f_0 \in C_0^\infty(\Sigma)$. We have

$$(f|b^{-2}f)_{\mathrm{en}} = (g|g)_{\mathrm{en}} = \|f_0\|^2_{\tilde{\mathcal{H}}} + (f_1 - \mathrm{i}\tilde{w}^*f_0|\tilde{h}^{-1}(f_1 - \mathrm{i}\tilde{w}^*f_0))_{\tilde{\mathcal{H}}} < \infty,$$

since $f_1 - \mathrm{i}\tilde{w}^*f_0 \in C_0^\infty(\Sigma) \subset \mathrm{Dom}\,\tilde{h}^{-\frac{1}{2}}$. Therefore, (9.10) is satisfied and one can define ground and thermal states $\tilde{\omega}_\beta$, $\beta \in]0,\infty]$ for $\tilde{P}$, whose covariances, denoted by $\tilde{\lambda}^\pm_\beta$ are introduced in Definitions 9.1.4 and 9.1.5.

It is now easy to define the vacuum and thermal states for P, since by (9.27) $Z : (C_0^\infty(\Sigma;\mathbb{C}^2),\tilde{q}) \to (C_0^\infty(\Sigma;\mathbb{C}^2),q)$ is unitary.

Definition 9.5.1. *The* ground state ω_∞ *associated to the Killing vector field* X *is the quasi-free state on* $\mathrm{CCR}^{\mathrm{pol}}(C_0^\infty(\Sigma;\mathbb{C}^2),q)$ *defined by the covariances*

$$\lambda^\pm_\infty = (Z^{-1})^*\tilde{\lambda}_\infty Z^{-1}. \tag{9.29}$$

The state ω_∞ is a pure state.

DEFINITION 9.5.2. *The* β-KMS state ω_β *associated to the Killing vector field* X *is the quasi-free state on* $\mathrm{CCR}^{\mathrm{pol}}(|b|C_0^\infty(\Sigma;\mathbb{C}^2),q)$ *defined by the covariances*

$$\lambda_\beta^\pm = (Z^{-1})^* \tilde{\lambda}_\infty Z^{-1}. \tag{9.30}$$

The state ω_β is not a pure state.

REMARK 9.5.3. *If the shift vector field* w *vanishes, then the spacetime* (M,g) *is static and the reduction in Section 9.4 produces an abstract Klein-Gordon operator* $\tilde{P}$ *of the form considered in Subsection 4.10.3. The formulas giving* $\lambda_\infty^\pm$ *and* $\lambda_\beta^\pm$ *simplify greatly using* (4.46), (4.49).

9.6. Hadamard property

In this subsection we prove that ω_β, $\beta \in]0,+\infty]$ are Hadamard states, a result due to Sahlmann and Verch [**SV1**].

THEOREM 9.6.1. *The states* ω_β *with* $\beta \in]0,+\infty]$ *are Hadamard states.*

Proof. Let $\Lambda_\beta^\pm \in \mathcal{D}'(M\times M)$ be the spacetime covariances of ω_β for $0<\beta\leq\infty$. In the Killing time coordinates (t,y) we have $\Lambda_\beta^\pm(t_1,t_2,y_1,y_2) = T_\beta^\pm(t_1-t_2,y_1,y_2)$, with $T_\beta^\pm \in \mathcal{D}'(\mathbb{R}\times\Sigma\times\Sigma)$, since ω_β is τ_t invariant.

From the ground state or KMS condition, it follows that there exist $F_\beta^\pm : \mathbb{R}\pm\mathrm{i}\,]0,\beta[\to\mathcal{D}'(\Sigma\times\Sigma)$ holomorphic such that $T_\beta^\pm(t,y_1,y_2) = F_\beta^\pm(t\pm\mathrm{i}0,y_1,y_2)$. By Proposition 7.1.5, we obtain that

$$\mathrm{WF}(T_\beta^\pm) \subset \{\pm\tau>0\}.$$

Applying then the results on the pullback of distributions in 7.2.4 we see that

$$\mathrm{WF}(\Lambda_\beta^\pm)' \subset \{\pm\tau_1>0\}\times\{\pm\tau_2>0\}.$$

Since $\mathrm{WF}(\Lambda_\beta^\pm)' \subset \mathcal{N}\times\mathcal{N}$, this implies that $\mathrm{WF}(\Lambda_\beta^\pm)' \subset \mathcal{N}^+\times\mathcal{N}^+$, using that $X=\frac{\partial}{\partial t}$ is future directed time-like. □

CHAPTER 10

Pseudodifferential calculus on manifolds

In this chapter we describe various versions of *pseudodifferential calculus* on manifolds. The pseudodifferential calculus is a standard tool in microlocal analysis, but it is also useful for the global analysis of partial differential equations on smooth manifolds. Of particular interest to us is the *Shubin calculus*, which is a global calculus on non compact manifolds relying on the notion of *bounded geometry*. Its two important properties are the *Seeley* and *Egorov theorems*.

In applications to quantum field theory the manifold is taken to be a Cauchy surface Σ in a spacetime (M, g). It turns out that the Cauchy surface covariances of pure Hadamard states can be constructed as pseudodifferential operators on Σ. This will be treated in detail in Chapter 11.

10.1. Pseudodifferential calculus on $\mathbb{R}^n$

We now recall standard facts about the *uniform pseudodifferential calculus* on $\mathbb{R}^n$. We refer the reader to [**H3**, Section 18.1] or [**Sh1**, Chap. 4] for details.

10.1.1. Symbol classes. Let $U \subset \mathbb{R}^n$ an open set. We denote by $S^m(T^*U)$, $m \in \mathbb{R}$ the symbol class defined by:

(10.1)
$$a \in S^m(T^*U) \text{ if } |\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \leq C_{\alpha\beta}(\langle\xi\rangle^{m-|\beta|}),\ \forall\ \alpha,\beta \in \mathbb{N}^d,\ (x,\xi) \in T^*U.$$

We denote by $S^m_{\rm h}(T^*U)$ the subspace of $S^m(T^*U)$ of symbols *homogeneous* of degree m in the ξ variable (outside a neighborhood of the origin)

(10.2)
$$a \in S^m_{\rm h}(T^*U) \text{ if } a \in S^m(T^*U) \text{ and } a(x,\lambda\xi) = \lambda^m a(x,\xi),\ \lambda \geq 1,\ |\xi| \geq 1.$$

If $a_{m-k} \in S^{m-k}(T^*U)$ for $k \in \mathbb{N}$ and $a \in S^m(T^*U)$ we write

$$a \sim \sum_{k=0}^{\infty} a_{m-k}$$

if

(10.3)
$$r_{m-n-1}(a) = a - \sum_{k=0}^{n} a_{m-k} \in S^{m-n-1}(T^*U),\ \forall\ n \in \mathbb{N}.$$

If $a_{m-k} \in S^{m-k}(T^*U)$ for $k \in \mathbb{N}$, then there exists $a \in S^m(T^*U)$, unique modulo $S^{-\infty}(T^*U)$, such that $a \sim \sum_{k=0}^{\infty} a_{m-k}$.

We say that a symbol $a \in S^m(T^*U)$ is *poly-homogeneous* if $a \sim \sum_{k=0}^{\infty} a_{m-k}$ for $a_{m-k} \in S^{m-k}_{\rm h}(T^*U)$. The symbols a_{m-k} are then clearly unique modulo $S^{-\infty}(T^*U)$. The subspace of *poly-homogeneous symbols* of degree m will be denoted by $S^m_{\rm ph}(T^*U)$.

We equip $S^m(T^*U)$ with the Fréchet space topology given by the semi-norms

$$\|a\|_{m,N} := \sup_{|\alpha|+|\beta|\leq N,(x,\xi)\in T^*U} |\langle\xi\rangle^{-m+|\beta|}\partial_x^\alpha\partial_\xi^\beta a|.$$

The topology of $S^m_{\rm ph}(T^*U)$ is a bit different: we equip $S^m_{\rm ph}(T^*U)$ with the seminorms of a_{m-k} in $S^{m-k}(T^*U)$ and of $r_{m-n-1}(a)$ in $S^{m-n-1}(T^*U)$, for $0 \le k \le n \in \mathbb{N}$, where a_{m-k} and $r_{m-n-1}(a)$ are defined in (10.3).

We set

$$S^\infty_{\rm (ph)}(T^*U) := \bigcup_{m\in\mathbb{R}} S^m_{\rm (ph)}(T^*U), \quad S^{-\infty}(T^*U) := \bigcap_{m\in\mathbb{R}} S^m(T^*U).$$

equipped with the inductive, resp. projective limit topology.

10.1.2. Principal part and characteristic set. The *principal part* of $a \in S^m(T^*\mathbb{R}^n)$, denoted by $\sigma_{\rm pr}(a)$, is the equivalence class of a in S^m/S^{m-1}. If $a \in S^m_{\rm ph}$, then $a + S^{m-1}$ has a unique representative in $S^m_{\rm h}$, namely the function a_m in (10.3). Therefore, in this case the principal part of a is a function on $T^*\mathbb{R}^n$, homogeneous of degree m in ξ.

The *characteristic set* of $a \in S^m_{\rm ph}$ is defined as

$$\mathrm{Char}(a) := \{(x,\xi) \in T^*\mathbb{R}^n \setminus o :\ a_m(x,\xi) = 0\}; \tag{10.4}$$

it is clearly conic in the ξ variable.

A symbol $a \in S^m(T^*\mathbb{R}^n)$ is *elliptic* if there exist $C, R > 0$ such that

$$|a(x,\xi)| \ge C\langle\xi\rangle^m, \quad |\xi| \ge R.$$

Clearly, $a \in S^m_{\rm ph}(T^*\mathbb{R}^n)$ is elliptic iff $\mathrm{Char}(a) = \emptyset$.

10.1.3. Pseudodifferential operators on $\mathbb{R}^n$. For $a \in S^m_{\rm ph}(T^*\mathbb{R}^n)$, we denote by $\mathrm{Op}(a)$ the *Kohn-Nirenberg quantization* of a, defined by

$$\mathrm{Op}(a)u(x) = a(x,D)u(x) := (2\pi)^{-n} \iint \mathrm{e}^{\mathrm{i}(x-y)\xi} a(x,\xi)u(y)\mathrm{d}y\mathrm{d}\xi, \quad u \in C^\infty_0(\mathbb{R}^n).$$

10.1.4. Mapping properties. Denote by $H^s(\mathbb{R}^n)$ the Sobolev space of order s and put

$$H^\infty(\mathbb{R}^n) := \bigcap_{s\in\mathbb{R}} H^s(\mathbb{R}^n), \quad H^{-\infty}(\mathbb{R}^n) := \bigcup_{s\in\mathbb{R}} H^s(\mathbb{R}^n)$$

Then if $a \in S^m_{\rm ph}(T^*\mathbb{R}^n)$ we have the continuous mapping

$$\mathrm{Op}(a) : H^s(\mathbb{R}^n) \longrightarrow H^{s-m}(\mathbb{R}^n),$$

hence $\mathrm{Op}(a) : H^\infty(\mathbb{R}^n) \to H^\infty(\mathbb{R}^n)$ and $\mathrm{Op}(a) : H^{-\infty}(\mathbb{R}^d) \to H^{-\infty}(\mathbb{R}^d)$.

We denote by $\Psi^m(\mathbb{R}^n)$ the space $\mathrm{Op}(S^m_{\rm ph}(T^*\mathbb{R}^n))$ and set

$$\Psi^\infty(\mathbb{R}^n) = \bigcup_{m\in\mathbb{R}} \Psi^m(\mathbb{R}^n), \quad \Psi^{-\infty}(\mathbb{R}^n) = \bigcap_{m\in\mathbb{R}} \Psi^m(\mathbb{R}^n).$$

We will often write Ψ^m instead of $\Psi^m(\mathbb{R}^n)$. We equip $\Psi^m(\mathbb{R}^n)$ with the Fréchet space topology obtained from the topology of $S^m_{\rm ph}(T^*\mathbb{R}^n)$.

10.1.5. Principal symbol. If $A = a(x,D_x) \in \Psi^m(\mathbb{R}^n)$, then the m-homogeneous function $\sigma_{\rm pr}(A) =: a_m(x,\xi)$ is called the *principal symbol* of A.

10.1.6. Composition and adjoint. If we equip $\Psi^\infty(\mathbb{R}^n)$ with the product and $*$ involution of $L(H^\infty(\mathbb{R}^n))$, then $\Psi^\infty(\mathbb{R}^n)$ is a graded $*$-algebra with

$$A^* \in \Psi^m(\mathbb{R}^n),\ A_1A_2 \in \Psi^{m_1+m_2}(\mathbb{R}^n),\ \text{for } A \in \Psi^m(\mathbb{R}^n),\ A_i \in \Psi^{m_i}(\mathbb{R}^n).$$

One has

$$\sigma_{\mathrm{pr}}(A^*) = \overline{\sigma_{\mathrm{pr}}(A)},\quad \sigma_{\mathrm{pr}}(A_1A_2) = \sigma_{\mathrm{pr}}(A_1)\sigma_{\mathrm{pr}}(A_2),$$
$$\sigma_{\mathrm{pr}}([A_1, A_2]) = \{\sigma_{\mathrm{pr}}(A_1), \sigma_{\mathrm{pr}}(A_2)\},$$

where $\{a, b\} = \partial_\xi a \cdot \partial_x b - \partial_x a \cdot \partial_\xi b$ is the Poisson bracket of a and b.

Let $s, m \in \mathbb{R}$. Then the map

$$S^m_{\mathrm{ph}}(T^*\mathbb{R}^n) \ni a \longmapsto \mathrm{Op}(a) \in B(H^s(\mathbb{R}^n), H^{s-m}(\mathbb{R}^n)) \tag{10.5}$$

is continuous.

10.1.7. Ellipticity. An operator $A \in \Psi^m$ is *elliptic* if its principal symbol $\sigma_{\mathrm{pr}}(A)$ is elliptic. If $A \in \Psi^m$ is elliptic, then there exists $B \in \Psi^{-m}$, unique modulo $\Psi^{-\infty}$, such that $AB - \mathbb{1}, BA - \mathbb{1} \in \Psi^{-\infty}$. Such an operator B is a parametrix of A in the sense of Definition 7.4.1. We denote it by $A^{(-1)}$.

10.1.8. Seeley's theorem. The uniform pseudodifferential calculus on $\mathbb{R}^n$ enjoys plenty of nice properties. For example, if $A \in \Psi^m(\mathbb{R}^n)$, $m > 0$ is elliptic, then A with domain $\mathrm{Dom}\, A = H^m(\mathbb{R}^n)$ is closed as an unbounded operator on $L^2(\mathbb{R}^n)$.

If $z \in \mathrm{res}(A)$, where $\mathrm{res}(A) \subset \mathbb{C}$ is the *resolvent set* of A, the resolvent $(A-z)^{-1}$ belongs to $\Psi^{-m}(\mathbb{R}^n)$ and its principal symbol equals $\sigma_{\mathrm{pr}}(A)^{-1}$. If moreover A is symmetric on $\mathcal{S}(\mathbb{R}^n)$, then it is selfadjoint on $H^m(\mathbb{R}^n)$. If $0 \in \mathrm{res}(A)$ then A^s for $s \in \mathbb{R}$ belongs to $\Psi^{ms}(\mathbb{R}^n)$ with principal symbol $\sigma_{\mathrm{pr}}(A)^s$. This last result is an example of *Seeley's theorem.*

10.2. Pseudodifferential operators on a manifold

The uniform pseudodifferential calculus transforms covariantly under local diffeomorphisms. This means that if $U_i \subset V_i$ are precompact open sets, $\psi = V_1 \to V_2$ is a diffeomorphism and $\chi_i \in C^\infty_0(V_i)$ with $\chi_i = 1$ on U_i, for $A \in \Psi^m(\mathbb{R}^n)$ one has

$$\chi_1 A \psi^*(\chi_2 u) = Bu,\ \ \forall u \in \mathcal{D}'(\mathbb{R}^n),$$

where $B \in \Psi^m(\mathbb{R}^n)$ and

$$\sigma_{\mathrm{pr}}(B)(x,\xi) = \sigma_{\mathrm{pr}}(A)(\psi(x), {}^tD\psi(x)^{-1}\xi),\quad (x,\xi) \in T^*U_1. \tag{10.6}$$

This allows to extend the pseudodifferential calculus to smooth manifolds. We follow the exposition in [**Sh1**, Chap. 1], [**H3**, Section 18.1].

10.2.1. Pseudodifferential calculus on a manifold. Let M be a smooth, n-dimensional manifold. Let $U \subset M$ be a precompact chart open set and $\psi : U \to \tilde{U}$ a chart diffeomorphism, where $\tilde{U} \subset \mathbb{R}^n$ is precompact, open. We denote by $\psi^* : C^\infty_0(\tilde{U}) \to C^\infty_0(U)$ the map defined by $\psi^* u(x) := u \circ \psi(x)$.

Definition 10.2.1. *A linear continuous map $A : C^\infty_0(M) \to C^\infty(M)$ belongs to $\Psi^m(M)$ if the following condition holds:*

Let $U \subset M$ be precompact open, $\psi : U \to \tilde{U}$ a chart diffeomorphism, $\chi_1, \chi_2 \in C^\infty_0(U)$ and $\tilde{\chi}_i = \chi_i \circ \psi^{-1}$. Then there exists $\tilde{A} \in \Psi^m(\mathbb{R}^n)$ such that

$$(\psi^*)^{-1}\chi_1 A \chi_2 \psi^* = \tilde{\chi}_1 \tilde{A} \tilde{\chi}_2. \tag{10.7}$$

The elements of $\Psi^m(M)$ are called (classical) pseudodifferential operators *of order m on M.*

The subspace of $\Psi^m(M)$ of pseudodifferential operators with properly supported kernels *is denoted by $\Psi^m_{\mathrm{c}}(M)$.*

We set

$$\Psi^{\infty}_{(\mathrm{c})}(M) := \bigcup_{m\in\mathbb{R}} \Psi^{m}_{(\mathrm{c})}(M).$$

We also denote by

$$\mathcal{R}^{-\infty}(M) := L(\mathcal{E}'(M), C^{\infty}(M))$$

the space of *smoothing operators*, or equivalently of operators with kernels in $C^{\infty}(M\times M)$.

If $A\in\Psi^{m}(M)$ there exists (many) $A_{\mathrm{c}}\in\Psi^{m}_{\mathrm{c}}(M)$ such that $A-A_{\mathrm{c}}\in\mathcal{R}^{-\infty}(M)$.

10.2.2. Mapping properties. If $A\in\Psi^{m}(M)$, then

$$A: H^{s}_{\mathrm{c}}(M)\longrightarrow H^{s-m}_{\mathrm{loc}}(M),\ \mathcal{E}'(M)\longrightarrow\mathcal{D}'(M),\ C^{\infty}_{0}(M)\longrightarrow C^{\infty}(M) \text{ continuously,}$$

while if $A\in\Psi^{m}_{\mathrm{c}}(M)$

$$A: \begin{array}{lll} H^{s}_{\mathrm{c}}(M)\longrightarrow H^{s-m}_{\mathrm{c}}(M), & \mathcal{E}'(M)\longrightarrow\mathcal{E}'(M), & C^{\infty}_{0}(M)\longrightarrow C^{\infty}_{0}(M),\\ H^{s}_{\mathrm{loc}}(M)\longrightarrow H^{s-m}_{\mathrm{loc}}(M), & \mathcal{D}'(M)\longrightarrow\mathcal{D}'(M), & C^{\infty}(M)\longrightarrow C^{\infty}(M), \end{array}$$

where $H^{s}_{\mathrm{loc}}(M)$, resp. $H^{s}_{\mathrm{c}}(M)$ are the local, resp. compactly supported Sobolev spaces on M.

10.2.3. Principal symbol. From (10.6) and (10.7) it follows that to $A\in\Psi^{m}(M)$ one can associate its *principal symbol* $\sigma_{\mathrm{pr}}(A)\in C^{\infty}(T^{*}M\setminus o)$, which is homogeneous of degree m in the fiber variable ξ in $T^{*}_{x}M$, in $\{|\xi|\geq 1\}$. The operator A is called *elliptic* in $\Psi^{m}(M)$ at $X_0\in T^{*}M\setminus o$ if $\sigma_{\mathrm{pr}}(A)(X_0)\neq 0$.

10.2.4. Composition and adjoint. Note that if $\Psi^{\infty}_{(\mathrm{c})}(M) := \bigcup_{m\in\mathbb{R}}\Psi^{m}_{(\mathrm{c})}(M)$, then $\Psi^{\infty}_{\mathrm{c}}(M)$ is an algebra, but $\Psi^{\infty}(M)$ is not, since without the proper support condition, pseudodifferential operators cannot in general be composed. Of course, if M is compact, then $\Psi^{\infty}(M)=\Psi^{\infty}_{\mathrm{c}}(M)$, so this problem disappears.

If we fix a smooth density $d\mu$ on M, then we can define the adjoint A^{*} of $A\in\Psi^{\infty}_{\mathrm{c}}(M)$. Then $\Psi^{\infty}_{\mathrm{c}}(M)$ is a graded $*$-algebra with

$$A^{*}\in\Psi^{m}_{\mathrm{c}}(M),\ A_1A_2\in\Psi^{m_1+m_2}_{\mathrm{c}}(M),\quad \text{for } A\in\Psi^{m}_{\mathrm{c}}(M),\ A_i\in\Psi^{m_i}_{\mathrm{c}}(M).$$

One has

$$\sigma_{\mathrm{pr}}(A^{*})=\overline{\sigma_{\mathrm{pr}}(A)},\quad \sigma_{\mathrm{pr}}(A_1A_2)=\sigma_{\mathrm{pr}}(A_1)\sigma_{\mathrm{pr}}(A_2),$$
$$\sigma_{\mathrm{pr}}([A_1,A_2])=\{\sigma_{\mathrm{pr}}(A_1),\sigma_{\mathrm{pr}}(A_2)\},$$

where $\{a,b\}$ is again the Poisson bracket of a and b.

10.2.5. Ellipticity. For $A\in\Psi^{m}(M)$ we set

$$\mathrm{Char}(A) := \{X\in T^{*}M\setminus o : \sigma_{\mathrm{pr}}(A)(X)=0\},$$

which is a closed, conic subset of $T^{*}M\setminus o$, called the *characteristic set of* A. If $X_0\notin\mathrm{Char}(A)$ one says that A is *elliptic* at X_0. If $\mathrm{Char}(A)=\emptyset$, we say that A is *elliptic* in $\Psi^{m}(M)$.

An elliptic operator $A\in\Psi^{m}(M)$ has properly supported parametrices $B\in\Psi^{-m}_{\mathrm{c}}(M)$, unique modulo $\mathcal{R}^{-\infty}(M)$ such that $AB-\mathbb{1},\mathbb{1}-AB\in\mathcal{R}^{-\infty}(M)$. Again such a parametrix will be denoted by $A^{(-1)}$.

The *essential support* $\mathrm{essupp}(A)$ of $A\in\Psi^{\infty}(M)$ is the closed conic subset of $T^{*}X\setminus o$ defined by $X_0\notin\mathrm{essupp}(A)$ if there exists $B\in\Psi^{\infty}_{\mathrm{c}}(M)$ *elliptic* at X_0 such that $A\circ B$ is smoothing.

10.2.6. The wavefront set. It is well known that the wavefront set of distributions on M can be characterized by means of pseudodifferential operators. We summarize this type of results in the next proposition.

PROPOSITION 10.2.2. (1) *Let $u \in \mathcal{D}'(M)$, $X_0 \in T^*M \setminus o$. Then $X_0 \notin \mathrm{WF}u$ iff there exists $A \in \Psi^0_{\mathrm{c}}(M)$,* elliptic *at X_0 such that $Au \in C^\infty(M)$.*
(2) *Let $A \in \Psi^\infty(M)$. Then*

$$\mathrm{WF}(A)' = \{(X, X) : X \in \mathrm{essupp}(A)\}.$$

(3) *Let $K : C^\infty_0(M_1) \to \mathcal{D}'(M_2)$. Then $(X_1, X_2) \notin \mathrm{WF}(K)'$ for $X_i \in T^*M_i \setminus o_i$ iff there exists $A_i \in \Psi^0_{\mathrm{c}}(M_i)$, elliptic at X_i such that $A_1 K A_2$ is smoothing.*

The above pseudodifferential calculus is sufficient for a large part of microlocal analysis, as long as we study distributions only *microlocally*, i.e. if near $X_0 \in T^*M \setminus o$ we identify two distributions u_1 and u_2 if $X_0 \notin \mathrm{WF}(u_1 - u_2)$.

However, it is not sufficient for more advanced topics. For example, if M is equipped with a complete Riemannian metric h, the Laplace-Beltrami operator $-\Delta_h$ is elliptic in $\Psi^2_{\mathrm{c}}(M)$, with principal symbol $\xi \cdot h^{-1}(x)\xi$. It is also essentially selfadjoint on $C^\infty_0(M)$. One can show that its resolvent $(-\Delta_h + \mathrm{i})^{-1}$ does not belong to $\Psi^{-2}_{\mathrm{c}}(M)$, but only to $\Psi^{-2}(M)$.

So if M is not compact, one needs an intermediate calculus, lying between $\Psi^\infty_{\mathrm{c}}(M)$ and $\Psi^\infty(M)$, which is large enough to be stable under taking resolvents, and small enough to remain a $*$-algebra. There are many possible choices, essentially determined by the behavior of symbols near infinity in M. One of them is *Shubin's calculus*, **[Sh2]**, which relies on the notion of *bounded geometry*.

This calculus turns out to be sufficient for constructing Hadamard states on many physically relevant spacetimes, like cosmological spacetimes, Kerr, Kerr-de Sitter, Kerr-Kruskal spacetimes, or cones, double cones and wedges in Minkowski spacetime, see Section 11.7.

10.3. Riemannian manifolds of bounded geometry

The notion of a Riemannian manifold (M, g) of bounded geometry was introduced by Gromov, see e.g. **[CG]**, **[Ro]**. For our purposes the only use of the metric g is to provide local coordinates near any $x \in M$, namely the normal coordinates at x, and to equip the spaces of sections of tensors on M with Euclidean norms. Therefore we will use an alternative definition of bounded geometry, which is easier to check in practice.

We denote by δ the flat metric on $\mathbb{R}^n$ and by $B_n(y, r) \subset \mathbb{R}^n$ the open ball of center y and radius r. If $U \subset \mathbb{R}^n$ is open, we denote by $BT^p_q(U, \delta)$ the space of smooth (q, p) tensors on U, bounded together with all their derivatives on U. We equip $BT^p_q(U, \delta)$ with its Fréchet space topology. For $q = p = 0$ we obtain the space $C^\infty_{\mathrm{b}}(U)$ of smooth functions bounded together with all their derivatives.

DEFINITION 10.3.1. *A Riemannian manifold (M, g) is of* bounded geometry *if for each $x \in M$, there exist an open neighborhood U_x of x and a smooth diffeomorphism*

$$\psi_x : U_x \xrightarrow{\sim} B_n(0, 1)$$

with $\psi_x(x) = 0$, such that if $g_x := (\psi_x^{-1})^* g$, then
(1) *the family $\{g_x\}_{x \in M}$ is bounded in $BT^0_2(B_n(0, 1), \delta)$,*
(2) *there exists $c > 0$ such that $c^{-1}\delta \leq g_x \leq c\delta$, $x \in M$.*
A family $\{U_x\}_{x \in M}$ resp. $\{\psi_x\}_{x \in M}$ as above will be called a family of bounded chart neighborhoods*, resp.* bounded chart diffeomorphisms*.*

One can show, see e.g. [**GOW**, Theorem 2.4] that Definition 10.3.1 is equivalent to the usual definition, which requires that the injectivity radius $r = \inf_{x\in M} r_x$ is strictly positive and that $(\nabla^g)^k R_g$ is a bounded tensor for all $k \in \mathbb{N}$, where R_g and ∇^g are the Riemann curvature tensor and Levi-Civita connection associated to g. Here the norm on (q,p)-tensors is the norm inherited from the metric g. The canonical choice of U_x, ψ_x is as follows: one fixes for all $x \in M$ a linear isometry $e_x : (\mathbb{R}^n, \delta) \to (T_xM, g(x))$ and sets

$$U_x = B^g_M(x, r/2), \quad \psi_x^{-1}(v) = \exp^g_x((r/2)e_x v), \quad v \in B_n(0,1),$$

where $B^g_M(x,r)$ is the geodesic ball of center x and radius r and $\exp^g_x : B^{g(x)}_{T_xM}(0, r_x) \to M$ the exponential map at x.

10.3.1. Atlases and partitions of unity. It is known (see [**Sh2**, Lemma 1.2]) that if (M,g) is of bounded geometry, there exist coverings by bounded chart neighborhoods

$$M = \bigcup_{i\in\mathbb{N}} U_i, \quad U_i = U_{x_i}, \quad x_i \in M,$$

which in addition are *uniformly finite*, i.e. there exists $N \in \mathbb{N}$ such that $\bigcap_{i\in I} U_i = \emptyset$ if $\sharp I > N$. Setting $\psi_i = \psi_{x_i}$, we will call $\{U_i, \psi_i\}_{i\in\mathbb{N}}$ a *bounded atlas* of M. One can associate (see [**Sh2**, Lemma 1.3]) to a bounded atlas a partition of unity

$$1 = \sum_{i\in\mathbb{N}} \chi_i^2, \ \chi_i \in C^\infty_0(U_i)$$

such that $\{(\psi_i^{-1})^*\chi_i\}_{i\in\mathbb{N}}$ is a bounded sequence in $C^\infty_{\mathrm{b}}(B_n(0,1))$. Such a partition of unity will be called a *bounded partition of unity*.

10.3.2. Bounded tensors. We now recall the definition of *bounded tensors* on a manifold (M,g) of bounded geometry, see [**Sh2**].

Definition 10.3.2. *Let (M,g) be of bounded geometry. We denote by $BT^p_q(M,g)$ the spaces of smooth (q,p) tensors T on M such that if $T_x = (\psi_x^{-1})^*T$, then the family $\{T_x\}_{x\in M}$ is* bounded *in $BT^p_q(B_n(0,1))$. We equip $BT^p_q(M,g)$ with its natural Fréchet space topology.*

The Fréchet space topology on $BT^p_q(M,g)$ is independent on the choice of the family of bounded chart diffeomorphisms $\{\psi_x\}_{x\in M}$.

10.3.3. Bounded differential operators. For $m \in \mathbb{N}$ we denote by $\mathrm{Diff}^m_{\mathrm{b}}(B_n(0,1))$ the Fréchet space of m-th order differential operators on $B_n(0,1)$ with $C^\infty_{\mathrm{b}}(B_n(0,1))$ coefficients. We denote by $\mathrm{Diff}_{\mathrm{b}}(M)$ the space of m-th order differential operators on M such that if $P_x = (\psi_x^{-1})^*P$, then the family $\{P_x\}_{x\in M}$ is bounded in $\mathrm{Diff}^m_{\mathrm{b}}(B_n(0,1))$.

10.3.4. Sobolev spaces. Let $-\Delta_g$ be the Laplace-Beltrami operator on (M,g), defined as the closure of its restriction to $C^\infty_0(M)$.

Definition 10.3.3. *For $s \in \mathbb{R}$ we define the* Sobolev space $H^s(M,g)$ *as*

$$H^s(M,g) := \langle -\Delta_g\rangle^{-s/2} L^2(M, dVol_g),$$

with its natural Hilbert space topology.

One sets

$$H^\infty(M,g) := \bigcap_{m\in\mathbb{R}} H^s(M;g), \quad H^{-\infty}(M,g) := \bigcup_{m\in\mathbb{R}} H^s(M,g),$$

equipped with the inductive, resp. projective limit topology.

It is known (see e.g. [**Kr**, Section 3.3]) that if $\{U_i, \psi_i\}_{i\in\mathbb{N}}$ is a bounded atlas and $1 = \sum_i \chi_i^2$ is a subordinate bounded partition of unity, then an equivalent norm on $H^s(M,g)$ is given by

$$\|u\|_s^2 = \sum_{i\in\mathbb{N}} \|(\psi_i^{-1})^*\chi_i u\|^2_{H^s(B_n(0,1))}. \tag{10.8}$$

10.3.5. Equivalence classes of Riemannian metrics. If g' is another Riemannian metric on M, we write $g' \sim g$ if $g' \in BT_2^0(M,g)$ and $(g')^{-1} \in BT_0^2(M,g)$. One can show, see [**GOW**, Section 2.5], that then (M,g') is also of bounded geometry, that $BT_q^p(M,g) = BT_q^p(M,g')$ and $H^s(M,g) = H^s(M,g')$ as topological vector spaces, and that $\sim$ is an equivalence relation.

10.3.6. Examples. Compact Riemannian manifolds are clearly of bounded geometry, as are compact perturbations of Riemannian manifolds of bounded geometry.

Gluing two Riemannian manifolds of bounded geometry along a compact region or taking their cartesian product produces again a Riemannian manifold of bounded geometry.

If (K,h) is of bounded geometry, then the *warped product* $(\mathbb{R}_s \times K, g)$ for $g = ds^2 + F^2(s)h$ is of bounded geometry if

$$F(s) \geq c_0 > 0,\ \forall s \in \mathbb{R} \text{ for some } c_0 > 0,$$
$$|F^{(k)}(s)| \leq c_k F(s),\ \forall s \in \mathbb{R},\ k \geq 1,$$

see [**GOW**, Proposition 2.13].

10.4. The Shubin calculus

We now define the Shubin pseudodifferential calculus, see [**Sh2**], [**Kr**], which is a version of the uniform calculus of Section 10.1, adapted to manifolds of bounded geometry. We fix a manifold (M,g) of bounded geometry.

10.4.1. Symbol classes. Let us first define the symbol classes of Shubin's calculus. Recall that the topology of $S^m_{\mathrm{ph}}(T^*B_n(0,1))$ was defined in Subsection 10.1.1.

Definition 10.4.1. *We denote by $BS^m_{\mathrm{ph}}(T^*M)$ the space of all $a \in C^\infty(T^*M)$ such that for each $x \in M$, $a_x := (\psi_x^{-1})^*a \in S^m_{\mathrm{ph}}(T^*B_n(0,1))$ and the family $\{a_x\}_{x\in M}$ is* bounded *in $S^m_{\mathrm{ph}}(T^*B_n(0,1))$. We equip $BS^m_{\mathrm{ph}}(T^*M)$ with the semi-norms*

$$\|a\|_{m,i,p,\alpha,\beta} = \sup_{x\in M} \|a_x\|_{m,i,p,\alpha,\beta},$$

where $\|\cdot\|_{m,i,p,\alpha,\beta}$ are the semi-norms defining the topology of $S^m_{\mathrm{ph}}(T^*B_n(0,1))$.

The definition of $BS^m_{\mathrm{ph}}(T^*M)$ and its Fréchet space topology is independent of the choice of the atlas $\{U_x, \psi_x\}_{x\in M}$ with the above properties. As usual, we set

$$BS^\infty_{\mathrm{ph}}(T^*M) = \bigcup_{m\in\mathbb{R}} BS^m_{\mathrm{ph}}(T^*M).$$

A symbol $a \in BS^m_{\mathrm{ph}}(T^*M)$ has a principal part $a_m \in BS^m_{\mathrm{h}}(T^*M)$ which is homogeneous of degree m in the fiber variables.

A symbol $a \in BS^m_{\mathrm{ph}}(T^*M)$ is *elliptic* if there exists $C, R > 0$ such that

$$|a_x(y,\eta)| \geq C|\eta|^m,\ \ \forall x \in M,\ (y,\eta) \in T^*B_n(0,1),$$

hence ellipticity in $BS^m_{\mathrm{ph}}(T^*M)$ means *uniform* ellipticity.

10.4.2. Pseudodifferential operators. Let $\{U_i, \psi_i\}_{i\in\mathbb{N}}$ be a bounded atlas of M and

$$\sum_{i\in\mathbb{N}} \chi_i^2 = \mathbb{1}$$

a subordinate bounded partition of unity, see Subsection 10.3.1. Let

$$(\psi_i^{-1})^* dVol_g =: m_i dx,$$

so that $\{m_i\}_{i\in\mathbb{N}}$ is bounded in $C^\infty_{\rm b}(B_n(0,1))$. We set also

$$T_i : \quad L^2(U_i, dVol_g) \longrightarrow L^2(B_n(0,1), dx),$$

$$u \longmapsto m_i^{\frac{1}{2}} (\psi_i^{-1})^* u,$$

so that $T_i : L^2(U_i, dVol_g) \to L^2(B_n(0,1), dx)$ is unitary.

Definition 10.4.2. *Let $a \in BS^m(T^*M)$. We set*

$$\mathrm{Op}(a) := \sum_{i\in\mathbb{N}} \chi_i T_i^* \circ \mathrm{Op}(Ea_i) \circ T_i \chi_i,$$

where $a_i = a_{x_i}$ (see Definition 10.4.1*), and $E : S^m_{\rm ph}(T^*B(0,1)) \to S^m_{\rm ph}(T^*\mathbb{R}^n)$ is an extension map.*

Such a map Op constructed by means of a bounded atlas and a bounded partition of unity will be called a *bounded quantization map*.

Note that if $a \in BS^\infty_{\rm ph}(T^*M)$, then the distributional kernel of $\mathrm{Op}(a)$ is supported in

$$\{(x,y) \in M \times M : \ d(x,y) \leq C\},$$

for some $C > 0$, where d is the geodesic distance on M. In particular, $\mathrm{Op}(a) \in \Psi^\infty_{\rm c}(M)$, hence such operators can be composed. However, because of the above support property, $\mathrm{Op}(S^\infty_{\rm c}(T^*M))$ is not stable under composition.

To obtain an algebra of operators, it is necessary to add to $\mathrm{Op}(BS^\infty_{\rm ph}(T^*M))$ an ideal of smoothing operators, which we introduce below. In the sequel the Sobolev spaces $H^s(M,g)$ will be simply denoted by $H^s(M)$.

Definition 10.4.3. *We set*

$$\mathcal{W}^{-\infty}(M) := \bigcap_{m\in\mathbb{N}} B(H^{-m}(M), H^m(M)),$$

equipped with its natural topology given by the semi-norms

$$\|A\|_m = \|(-\Delta_g + 1)^{m/2} A (-\Delta_g + 1)^{m/2}\|_{B(L^2(M))}.$$

Note that $\mathcal{W}^{-\infty}(M)$ is strictly included in the ideal $\mathcal{R}^{-\infty}(M)$ of smoothing operators.

The next result shows the independence modulo $W^{-\infty}(M)$ of $\mathrm{Op}(BS^\infty(T^*M))$ on the above choices of $\{U_i, \psi_i, E, \chi_i\}$.

Proposition 10.4.4. *Let Op' be another bounded quantization map. Then*

$$\mathrm{Op} - \mathrm{Op}' : BS^\infty_{\rm ph}(T^*M) \longrightarrow \mathcal{W}^{-\infty}(M).$$

is continuous.

Definition 10.4.5. *We set for $m \in \mathbb{R} \cup \{\infty\}$:*

$$\Psi^m_{\rm b}(M) := \mathrm{Op}(BS^m_{\rm ph}(T^*M)) + \mathcal{W}^{-\infty}(M).$$

Clearly, $\Psi^m_{\rm c}(M) \subset \Psi^m_{\rm b}(M) \subset \Psi^m(M)$.

One can show that

$$\Psi^m_{\rm b}(M) : H^s(M) \longrightarrow H^{s-m}(M), \text{ continuously for } s \in \mathbb{R} \cup \{\pm\infty\}.$$

10.4.3. Composition and adjoint. To $A \in \Psi_{\mathrm{b}}^m(M)$ one can associate its *principal symbol* $\sigma_{\mathrm{pr}}(A) \in C^\infty(T^*M \setminus o)$, which is homogeneous of degree m on the fibers.

Again, A is *elliptic* in $\Psi_{\mathrm{b}}^m(M)$ if $\sigma_{\mathrm{pr}}(A)$ is elliptic in the sense of Subsection 10.4.1. An elliptic operator $A \in \Psi_{\mathrm{b}}^m(M)$ has parametrices $B \in \Psi_{\mathrm{b}}^{-m}(M)$, unique modulo $\mathcal{W}^{-\infty}(M)$ such that $AB - \mathbb{1}, \mathbb{1} - AB \in \mathcal{W}^{-\infty}(M)$. As before, such a parametrix will be denoted by $A^{(-1)}$. If we equip M with the density $dVol_g$, then we can define the adjoint A^* of $A \in \Psi_{\mathrm{b}}^\infty(M)$. Then $\Psi_{\mathrm{b}}^\infty(M)$ is a graded $*$-algebra with

$$A^* \in \Psi_{\mathrm{b}}^m(M),\ A_1A_2 \in \Psi_{\mathrm{b}}^{m_1+m_2}(M),\ \text{ for } A \in \Psi_{\mathrm{b}}^m(M),\ A_i \in \Psi_{\mathrm{b}}^{m_i}(M).$$

We have

$$\sigma_{\mathrm{pr}}(A^*) = \overline{\sigma_{\mathrm{pr}}(A)}, \quad \sigma_{\mathrm{pr}}(A_1A_2) = \sigma_{\mathrm{pr}}(A_1)\sigma_{\mathrm{pr}}(A_2),$$
$$\sigma_{\mathrm{pr}}([A_1, A_2]) = \{\sigma_{\mathrm{pr}}(A_1), \sigma_{\mathrm{pr}}(A_2)\},$$

where $\{a, b\}$ is the Poisson bracket of a and b. The results on adjoints are still true if $dVol_g$ is replaced by an arbitrary smooth, *bounded* density $d\mu$ on M.

10.5. Time-dependent pseudodifferential operators

We also need a time-dependent version of the calculus in Section 10.4, which we will briefly outline, referring to [**GOW**, Section 5] for details.

If $I \subset \mathbb{R}$ is an open interval and $\mathcal{F}$ is a Fréchet space whose topology is defined by the semi-norms $\|\cdot\|_n$, $n \in \mathbb{N}$, then the space $C_{\mathrm{b}}^\infty(I; \mathcal{F})$ is also a Fréchet space, with semi-norms $\sup_{t\in I} \|\partial_t^k f(t)\|_n$, $k, n \in \mathbb{N}$.

One can define in this way the spaces $C_{\mathrm{b}}^\infty(I; BS_{\mathrm{ph}}^m(T^*M))$, $C_{\mathrm{b}}^\infty(I; \mathcal{W}^{-\infty}(M))$ and

$$C_{\mathrm{b}}^\infty(I; \Psi_{\mathrm{b}}^m(M)) := \mathrm{Op}(C_{\mathrm{b}}^\infty(I; BS_{\mathrm{ph}}^m(T^*M))) + C_{\mathrm{b}}^\infty(I; \mathcal{W}^{-\infty}(M)),$$

where Op refers of course to quantization in the (x, ξ) variables. An element A of $C_{\mathrm{b}}^\infty(I; \Psi_{\mathrm{b}}^m(M))$ will be usually denoted by $A(t)$. All the results in Section 10.4 extend naturally to the time-dependent situation.

10.6. Seeley's theorem

The most important property of the Shubin calculus is its invariance under complex powers, which was shown in [**ALNV**] and is an extension of a classical result of Seeley [**Se**]. We consider here the simpler case of real powers, see [**GOW**, Theorem 5.12]. The Hilbert space $L^2(M, dVol_g)$ is denoted simply by $L^2(M)$.

THEOREM 10.6.1. *Let $a = a(t) \in C_{\mathrm{b}}^\infty(I; \Psi_{\mathrm{b}}^m(M))$, be elliptic and symmetric on $C_0^\infty(I; H^\infty(M))$. Then a is selfadjoint with domain $L^2(I; H^m(M))$. If $a(t) \geq c\mathbb{1}$ for some $c > 0$ then $a^s(t) \in C_{\mathrm{b}}^\infty(I; \Psi_{\mathrm{b}}^{ms}(M))$ for all $s \in \mathbb{R}$ and*

$$\sigma_{\mathrm{pr}}(a^s)(t) = (\sigma_{\mathrm{pr}}(a))^s(t),\ t \in I.$$

10.7. Egorov's theorem

We now state another important property of the Shubin calculus, namely *Egorov's theorem*, see [**GOW**, Section 5.4]. Let us consider an operator $\epsilon(t) = \epsilon_1(t) + \epsilon_0(t)$, such that

$$\begin{aligned} &\epsilon_i(t) \in C_{\mathrm{b}}^\infty(I; \Psi_{\mathrm{b}}^i(M)), \quad i = 0, 1, \\ &\epsilon_1(t) \text{ is elliptic, symmetric and bounded from below on } H^\infty(M). \end{aligned} \tag{10.9}$$

By Theorem 10.6.1, $\epsilon_1(t)$ with domain $\operatorname{Dom}\epsilon(t) = H^1(M)$ is selfadjoint, hence $\epsilon(t)$ with the same domain is closed, with non-empty resolvent set. We denote by $\operatorname{Texp}\left(\mathrm{i}\int_s^t \epsilon(\sigma)d\sigma\right)$ the associated *propagator*, defined by

$$\text{(10.10)}\qquad \begin{cases} \dfrac{\partial}{\partial t}\operatorname{Texp}\left(\mathrm{i}\displaystyle\int_s^t \epsilon(\sigma)d\sigma\right) = \mathrm{i}\epsilon(t)\operatorname{Texp}\left(\mathrm{i}\displaystyle\int_s^t \epsilon(\sigma)d\sigma\right), \quad t,s\in I,\\ \dfrac{\partial}{\partial s}\operatorname{Texp}\left(\mathrm{i}\displaystyle\int_s^t \epsilon(\sigma)d\sigma\right) = -\mathrm{i}\operatorname{Texp}\left(\mathrm{i}\displaystyle\int_s^t \epsilon(\sigma)d\sigma\right)\epsilon(s), \quad t,s\in I,\\ \operatorname{Texp}\left(\mathrm{i}\displaystyle\int_s^s \epsilon(\sigma)d\sigma\right) = \mathbb{1}, \quad s\in I. \end{cases}$$

The notation Texp comes from the *time-ordered exponential*, which is the standard tool to solve (10.10) when $\epsilon(t)$ is bounded. The existence of $\operatorname{Texp}\left(\mathrm{i}\int_s^t \epsilon(\sigma)d\sigma\right)$ is a classic result of Kato, see **[SG]** for a recent summary.

THEOREM 10.7.1. *Let $a\in\Psi^m(M)$ and $\epsilon(t)$ satisfying* (10.9)*. Then*

$$a(t,s) := \operatorname{Texp}\left(\mathrm{i}\int_s^t \epsilon(\sigma)d\sigma\right) a \operatorname{Texp}\left(\mathrm{i}\int_t^s \epsilon(\sigma)d\sigma\right) \in C^\infty_{\mathrm{b}}(I^2,\Psi^m(M)).$$

Moreover,

$$\sigma_{\mathrm{pr}}(a)(t,s) = \sigma_{\mathrm{pr}}(a)\circ\Phi(s,t),$$

where $\Phi(t,s): T^*M\setminus o\to T^*M\setminus o$ is the flow of the time-dependent Hamiltonian $\sigma_{\mathrm{pr}}(\epsilon)(t)$.

One can show, see **[GOW**, Lemma 5.14], that $\operatorname{Texp}\left(\mathrm{i}\int_s^t \epsilon(\sigma)d\sigma\right)\in B(H^m(M))$ for $m\in\mathbb{R}\cup\{\pm\infty\}$, hence $a(t,s)$ above is well defined.

CHAPTER 11

Construction of Hadamard states by pseudodifferential calculus

In this chapter we explain the construction in [**GW1, GOW**] of pure Hadamard states using the global pseudodifferential calculus described in Chapter 10. These Hadamard states are constructed via their Cauchy surface covariances with respect to some fixed Cauchy surface Σ. It is important to assume that the normal geodesic flow, see Subsection 5.4.3, exists for some uniform time interval. This apparently strong condition can actually be considerably relaxed, since one can perform conformal transformations on the metric. For example the Kerr or Kerr-de Sitter exterior spacetimes and the Kerr-Kruskal spacetime can be treated by this method.

An interesting pair of notions that appears in this context is the one of Lorentzian metrics and Cauchy surfaces of *bounded geometry* , with respect to some reference Riemannian metric. If Σ and (M, g) are of bounded geometry, Klein-Gordon operators on (M, g) can be reduced to a simple model form, which fits into the framework of Chapter 10.

It is rather clear that the construction of Hadamard states is intimately related to *parametrices* for the Cauchy problem on Σ. Traditionally those parametrices are constructed as *Fourier integral operators*, using solutions of the eikonal and transport equations.

Since we need to control the conditions in Proposition 6.1.5 on Cauchy surface covariances, like for example positivity, we need a global construction of parametrices, and it turns out that an approach via time-ordered exponentials is more convenient and, we think, more elegant, see Section 11.3.

Our construction is also equivalent to a factorization of the Klein-Gordon operator as a product of two first-order pseudodifferential operators, which was already used by Junker [**J1, J2**], who gave the first construction of the Cauchy covariances of Hadamard states using pseudodifferential calculus. His constructions were however restricted to the case when Σ is compact.

11.1. Hadamard condition on Cauchy surface covariances

The Hadamard condition in Section 8.3 is formulated in terms of the spacetime covariances $\Lambda^{\pm}$. We need a condition in term of the Cauchy surface covariances $\lambda_{\Sigma}^{\pm}$ for a space-like Cauchy surface Σ. We recall that $U_{\Sigma} : \mathcal{E}'(\Sigma; \mathbb{C}^2) \to \mathcal{D}'_{\mathrm{sc}}(M)$ is the Cauchy evolution operator for P, see Theorem 5.5.3.

PROPOSITION 11.1.1. *Let $c^{\pm}$ be linear maps that are continuous from $C_0^{\infty}(\Sigma; \mathbb{C}^2)$ to $C^{\infty}(\Sigma; \mathbb{C}^2)$ and from $\mathcal{E}'(\Sigma; \mathbb{C}^2)$ to $\mathcal{D}'(\Sigma; \mathbb{C}^2)$, such that for some neighborhood U of Σ in M we have*

$$\mathrm{WF}(U_{\Sigma} \circ c^{\pm})' \subset \mathcal{N}^{\pm} \times (T^*\Sigma \setminus o), \text{ over } U.$$

Let

$$\Lambda^{\pm} = \pm(\varrho_{\Sigma} G)^* q_{\Sigma} c^{\pm} (\varrho_{\Sigma} G).$$

Then

$$\mathrm{WF}(\Lambda^{\pm})' \subset \mathcal{N}^{\pm} \times (T^*M \setminus o). \tag{11.1}$$

Proof. Clearly $\Lambda^\pm : C_0^\infty(M) \to \mathcal{D}'(M)$ are continuous. By Proposition 5.5.4, we have $U_\Sigma = \mathrm{i}^{-1}(\varrho_\Sigma G)^* q_\Sigma$, and so $\Lambda^\pm = \pm \mathrm{i}^{-1} U_\Sigma c^\pm(\varrho_\Sigma G)$. We apply Subsection 7.2.8 for $M_1 = U$, $M_2 = \Sigma$, $M_3 = M$, $K_1 = U_\Sigma c^\pm$, $K_2 = \varrho_\Sigma G$ and obtain (11.1), first over $U \times M$, and then over $M \times M$ by propagation of singularities, using that $P\Lambda^\pm = 0$. □

11.2. Model Klein-Gordon operators

We now describe a rather simple class of Klein-Gordon operators to which more complicated ones can be reduced.

We fix an $(n-1)$-dimensional Riemannian manifold (Σ, k_0) of bounded geometry and an open interval $I \subset \mathbb{R}$ with $0 \in I$. Let $I \ni t \mapsto h_t$ a time-dependent Riemannian metric on Σ such that $h_t \in C_b^\infty(I; BT_2^0(\Sigma, k_0))$ and $h_t^{-1} \in C_b^\infty(I; BT_0^2(\Sigma, k_0))$.

We equip $M = I \times \Sigma$ with the Lorentzian metric $g = -dt^2 + h_t(x)dx^2$ and consider a Klein-Gordon operator P on (M, g) such that moreover $P \in \mathrm{Diff}^2_{\mathrm{b}}(M, k)$ for $k = dt^2 + k_0 dx^2$.

It is easy to see that P is then of the form

$$P = \partial_t^2 + r(t,x)\partial_t + a(t,x,\partial_x), \tag{11.2}$$

where $a(t,x,\partial_x) \in C^\infty_{\mathrm{b}}(I; \mathrm{Diff}_{\mathrm{b}}(\Sigma; k_0))$ such that

$$\text{(i)} \quad \sigma_{\mathrm{pr}}(a)(t,x,\xi) = \xi \cdot h_t(x)\xi,$$
$$\text{(ii)} \quad a(t,x,\partial_x) = a^*(t,x,\partial_x),$$

where the adjoint is defined with respect to the time-dependent scalar product

$$(u|v)_t = \int_\Sigma \overline{u} v \, dVol_{h_t}, \tag{11.3}$$

and $r_t = |h_t|^{-\frac{1}{2}} \partial_t |h_t|^{\frac{1}{2}}$. The two energy shells for P are

$$\mathcal{N}^\pm = \{(t,x,\tau,\xi) : \tau = \pm(\xi \cdot h_t(x)\xi)^{\frac{1}{2}},\ \xi \neq 0\}.$$

We set $\Sigma_t = \{t\} \times \Sigma$ in M equipped with the density $dVol_{h_t}$.

11.2.1. Cauchy problem. It is usual to rewrite the Klein-Gordon equation

$$(\partial_t^2 + r(t)\partial_t + a(t))\phi(t) = 0$$

as a first-order system

$$\mathrm{i}^{-1}\partial_t \psi(t) = H(t)\psi(t), \quad \text{where } H(t) = \begin{pmatrix} 0 & \mathbb{1} \\ a(t) & \mathrm{i}r(t) \end{pmatrix}, \tag{11.4}$$

by setting

$$\psi(t) = \begin{pmatrix} \phi(t) \\ \mathrm{i}^{-1}\partial_t \phi(t) \end{pmatrix} =: \varrho_t \phi.$$

We denote by

$$\mathcal{U}_H(t,s) := \mathrm{Texp}\left(\mathrm{i}\int_s^t H(\sigma)d\sigma\right), \quad s,t \in I, \tag{11.5}$$

the evolution operator associated to $H(t)$. We equip $L^2(\Sigma_t; \mathbb{C}^2)$ with the time-dependent scalar product obtained from (11.3), by setting

$$(f|g)_t := \int_{\Sigma_t} \left(\overline{f}_1 g_1 + \overline{f}_0 g_0\right) dVol_{h_t}.$$

We will use it to define adjoints of linear operators and to identify sesquilinear forms on $L^2(\Sigma;\mathbb{C}^2)$ with linear operators. For

$$q := \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

we have

$$q = \mathcal{U}_H^*(s,t) q \mathcal{U}_H(s,t), \quad s,t \in I, \tag{11.6}$$

i.e. the evolution operator $\mathcal{U}_H(t,s)$ is *symplectic*.

11.3. Parametrices for the Cauchy problem

Let $U_0 : \mathcal{E}'(\Sigma;\mathbb{C}^2) \to \mathcal{D}'_{\mathrm{sc}}(M)$ be the *Cauchy evolution operator* for P, which solves

$$\begin{cases} PU_0 = 0, \\ \varrho_0 U_0 = \mathbb{1}. \end{cases} \tag{11.7}$$

We will construct a parametrix $\tilde{U}_0$ for (11.7) such that

$$\begin{cases} P\tilde{U}_0 = 0, \\ \varrho_0 \tilde{U}_0 = \mathbb{1}, \end{cases} \quad \text{modulo smoothing errors.}$$

The theory of *Fourier integral operators*, one of the important topics in microlocal analysis, originated from the construction of parametrices by Lax [**La**] and Ludwig [**Lu**] for the Cauchy problem for wave equations (or, more generally, strictly hyperbolic systems). It amounts to looking for $\tilde{U}_0$ as a sum of two oscillatory integrals

$$(2\pi)^{-d} \int \mathrm{e}^{\mathrm{i}(\varphi^{\pm}(t,x,\xi) - y\cdot\xi)} a^{\pm}(t,x,\xi) d\xi.$$

The phase functions $\varphi^{\pm}(t,x,\xi)$ are solutions of the *eikonal equation*

$$\begin{cases} (\partial_t \varphi^{\pm}(t,x,\xi))^2 - a(t,x,\partial_x \varphi^{\pm}(t,x,\xi)) = 0, \\ \varphi^{\pm}(0,x,\xi) = x\cdot\xi, \end{cases}$$

and the amplitudes $a^{\pm}(t,x,\xi)$ solve a first-order differential equation along the bicharacteristics of P.

It is actually simpler and more convenient to use a more operator theoretical approach. Instead, we will try to find time-dependent operators $b^{\pm}(t) \in C^{\infty}_{\mathrm{b}}(I;\Psi^1_{\mathrm{b}}(\Sigma))$ such that

$$\mathcal{U}^{\pm}(t) = \mathrm{Texp}\left(\mathrm{i}\int_0^t b^{\pm}(\sigma) d\sigma\right)$$

solve the equation

$$P\mathcal{U}^{\pm}(t) = 0, \ \text{ modulo smoothing errors.} \tag{11.8}$$

If we try to solve (11.8) exactly, we see that $b(t)$ should satisfy the *Riccati equation*

$$\mathrm{i}\partial_t b^{\pm} - (b^{\pm})^2 + a + \mathrm{i}r b^{\pm} = 0. \tag{11.9}$$

A straightforward computation shows that (11.9) is equivalent to a factorization

$$P = (\partial_t + \mathrm{i}b^{\pm} + r)(\partial_t - \mathrm{i}b^{\pm}). \tag{11.10}$$

Such a factorization was already used by Junker [**J1, J2**] to construct Hadamard states by pseudodifferential calculus, in the case where the Cauchy surface Σ is compact.

11.3.1. Solving the Riccati equation. We now explain how to solve (11.9), modulo smoothing errors. The first step consists in reducing the task to the case when $a(t) := a(t, x, \partial_x)$ is strictly positive, as an operator on $L^2(\Sigma, |h_t|^{\frac{1}{2}} dx)$.

One can find, see [**GOW**, Proposition 5.11], an operator $c_{-\infty}(t) \in C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma))$ and a constant $c > 0$ such that $a(t) + c_{-\infty}(t) \geq c\mathbb{1}$, for all $t \in I$. One sets then $\epsilon(t) := (a(t) + c_{-\infty}(t))^{\frac{1}{2}}$, which by Theorem 10.6.1 belongs to $C^\infty_{\rm b}(I; \Psi^1_{\rm b}(\Sigma))$, with principal symbol $(\xi \cdot h_t(x)\xi)^{\frac{1}{2}}$.

Proposition 11.3.1. *There exists an operator $b(t) \in C^\infty_{\rm b}(I; \Psi^1_{\rm b}(\Sigma))$, unique modulo $C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma))$, such that*

(i) $b(t) = \epsilon(t) + C^\infty_{\rm b}(I; \Psi^0_{\rm b}(\Sigma))$,

(ii) $(b(t) + b^*(t))^{-1} = (2\epsilon(t))^{-\frac{1}{2}}(\mathbb{1} + r_{-1})(2\epsilon(t))^{-\frac{1}{2}},\ r_{-1} \in C^\infty_{\rm b}(I; \Psi^{-1}_{\rm b}(\Sigma))$,

(iii) $(b(t) + b^*(t))^{-1} \geq c\epsilon(t)^{-1}$, *for some* $c > 0$,

(iv) $\mathrm{i}\partial_t b^\pm(t) - (b^\pm)^2(t) + a(t) + \mathrm{i}r(t)b^\pm(t) = r^\pm_{-\infty}(t) \in C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma))$,

for $b^+(t) := b(t),\ b^- := -b^*(t)$.

Proof. We follow the proof in [**GOW**, Theorem 6.1]. Discarding error terms in $C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma))$, we can assume that $\epsilon(t) = \mathrm{Op}(\hat\epsilon)(t)$, $\hat\epsilon(t) \in C^\infty_{\rm b}(I; BS^1_{\rm ph}(T^*\Sigma))$. We look for $b(t)$ of the form $b(t) = \epsilon(t) + d(t)$ for

$$d(t) = \mathrm{Op}(\hat d)(t), \quad \hat d(t) \in C^\infty_{\rm b}(I; BS^0_{\rm ph}(T^*\Sigma)).$$

Since $\epsilon(t)$ is elliptic, it admits a parametrix

$$\epsilon^{(-1)}(t) = \mathrm{Op}(\hat c)(t), \quad \hat c(t) \in C^\infty_{\rm b}(I; BS^{-1}_{\rm ph}(\Sigma)).$$

The equation (11.9) becomes, modulo error terms in $C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma))$,

$$d(t) = \frac{\mathrm{i}}{2}\Big(\epsilon^{(-1)}(t)\partial_t\epsilon(t) + \epsilon^{(-1)}(t)r(t)\epsilon(t)\Big) + F(d)(t), \tag{11.11}$$

with

$$F(d)(t) = \frac{1}{2}\epsilon^{(-1)}(t)\Big(\mathrm{i}\partial_t d(t) + [\epsilon(t), d(t)] + \mathrm{i}r(t)d(t) - d^2(t)\Big).$$

By means of symbolic calculus, we obtain that

$$F(d)(t) = \mathrm{Op}(\tilde F(\hat d))(t) + C^\infty_{\rm b}(I; \mathcal{W}^{-\infty}(\Sigma)),$$

with

$$\tilde F(\hat d)(t) = \frac{1}{2}\hat c(t)\sharp\Big(\mathrm{i}\partial_t\hat d(t) + \hat\epsilon(t)\sharp\hat d(t) - \hat d(t)\sharp\hat\epsilon(t) + \mathrm{i}r(t)\sharp\hat d(t) - \hat d(t)\sharp\hat d(t)\Big),$$

where the operation $\sharp$ (sometimes called the *Moyal product*) is defined by

$$\mathrm{Op}(a)\mathrm{Op}(b) = \mathrm{Op}(a\sharp b) \text{ modulo } BS^{-\infty}(\Sigma).$$

The equation (11.11) becomes

$$\hat d(t) = \hat d_0(t) + \tilde F(\hat d)(t), \tag{11.12}$$

for

$$\hat d_0(t) = \frac{\mathrm{i}}{2}\Big(\hat c(t)\sharp\partial_t\hat\epsilon(t) + \hat c(t)\sharp r(t)\sharp\hat\epsilon(t)\Big) \in C^\infty_{\rm b}(I; BS^0_{\rm ph}(T^*\Sigma)).$$

The map $\tilde F$ has the following property:

(11.13)
$$\hat d_1(t), \hat d_2(t) \in C^\infty_{\rm b}(I; BS^0_{\rm ph}(T^*\Sigma)), \quad \hat d_1(t) - \hat d_2(t) \in C^\infty_{\rm b}(I; BS^{-j}_{\rm ph}(T^*\Sigma))$$
$$\Longrightarrow \quad \tilde F(\hat d_1)(t) - \tilde F(\hat d_2)(t) \in C^\infty_{\rm b}(I; BS^{-j-1}_{\rm ph}(T^*\Sigma)).$$

This allows to solve (11.13) symbolically by setting

$$\hat{d}_{-1}(t) = 0,\ \hat{d}_n(t) := \hat{d}_0(t) + \tilde{F}(\hat{d}_{n-1})(t),$$

and

$$\hat{d}(t) \sim \sum_{n\in\mathbb{N}} \hat{d}_n(t) - \hat{d}_{n-1}(t),$$

which is an asymptotic series, since, by (11.13), $\hat{d}_n(t)-\hat{d}_{n-1}(t) \in C^\infty_{\mathrm{b}}(I; BS^{-n}_{\mathrm{ph}}(T^*\Sigma))$. It follows that $\epsilon(t) + d(t)$ solves (11.9) modulo $C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$, hence satisfies (i) and (iv) in the proposition.

In the rest of the proof $\epsilon(t)$ will again denote the square root $\epsilon(t) = (a(t) + c_{-\infty}(t))^{\frac{1}{2}}$, which differs from $\mathrm{Op}(\hat{\epsilon})(t)$ by an error in $C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$, so that $\epsilon(t) + d(t)$ still solves (11.9) modulo $C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$.

To satisfy (ii), (iii) we need to further modify $\epsilon(t) + d(t)$ by an error term in $C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$, which will not invalidate (i) and (iv). We set

$$s(t) = \epsilon(t) + d(t) + \epsilon^*(t) + d^*(t),$$

which is selfadjoint, with principal symbol equal to $2(\xi\cdot h_t^{-1}(x)\xi)^{\frac{1}{2}}$. By [**GOW**, Proposition 5.11], there exist an $r_{-\infty} \in C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$ and a constant $c > 0$ such that

$$c^{-1}\epsilon(t) \leq s(t) + r_{-\infty}(t) \leq c\epsilon(t), \quad t \in I. \tag{11.14}$$

Now set

$$b(t) := \epsilon(t) + d(t) + \frac{1}{2} r_{-\infty}(t).$$

Property (iii) follows from (11.14) and the Kato-Heinz theorem. To prove property (ii), we write

$$b(t) + b^*(t) = (2\epsilon)^{\frac{1}{2}}(t)(\mathbb{1} + \tilde{r}_{-1}(t))(2\epsilon)^{\frac{1}{2}}(t),$$

where $\tilde{r}_{-1}(t) \in C^\infty_{\mathrm{b}}(I; \Psi^{-1}_{\mathrm{b}}(\Sigma))$, by Theorem 10.6.1. Since $(\mathbb{1}+\tilde{r}_{-1})(t)$ is boundedly invertible, we have, again by Theorem 10.6.1, that

$$(\mathbb{1} + \tilde{r}_{-1})^{-1}(t) = \mathbb{1} + r_{-1}(t),\ r_{-1}(t) \in C^\infty_{\mathrm{b}}(I; \Psi^{-1}_{\mathrm{b}}(\Sigma)),$$

which implies (ii).

We observe then that if $b(t) \in C^\infty_{\mathrm{b}}(I; \Psi^\infty_{\mathrm{b}}(\Sigma))$ we have

$$(\partial_t b)^*(t) = \partial_t(b^*)(t) + r(t)b^*(t) - b^*(t)r(t).$$

Note that the adjoint is computed with respect to the time-dependent scalar product (11.3), so $(\partial_t b)^* \neq \partial_t(b^*)$. This implies that $-b^*(t)$ is also a solution of (11.9) modulo $C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma))$. The proof of the proposition is complete. □

11.3.2. Parametrices for the Cauchy problem. We can now construct parametrices for the Cauchy problem (11.7). In fact, if

$$u^\pm f = (b^+ - b^-)^{-1}(0)(\mp b^\mp(0) f_0 \pm f_1), \quad f \in H^\infty(\Sigma), \tag{11.15}$$

we obtain by an easy computation that

$$\tilde{U}_0 f(t) := \mathcal{U}^+(t)u^+ f + \mathcal{U}^-(t)u^- f \tag{11.16}$$

solves

$$\begin{cases} P\tilde{U}_0 \in C^\infty_{\mathrm{b}}(I; \mathcal{W}^{-\infty}(\Sigma)), \\ \varrho_0 \tilde{U}_0 = \mathbb{1}, \end{cases}$$

hence is a parametrix for the Cauchy problem (11.7).

11.3.3. Microlocal splitting of Cauchy data. It is easy to see that if $u \in H^\infty(\Sigma)$, then $\mathrm{WF}(\mathcal{U}^\pm(\cdot)u) \subset \mathcal{N}^\pm$. Therefore, if $f \in \operatorname{Ker} u^\mp$, one has also $\mathrm{WF}(U_0 f) \subset \mathcal{N}^\pm$.

It turns out that $\operatorname{Ker} u^\mp$ are complementary spaces, for example in $H^\infty(\Sigma;\mathbb{C}^2)$, which are moreover orthogonal with respect to q. This is summarized in the next proposition.

PROPOSITION 11.3.2. *Let*

$$T := \begin{pmatrix} \mathbb{1} & -\mathbb{1} \\ b^+(0) & -b^-(0) \end{pmatrix} (b^+ - b^-)^{-\frac{1}{2}}(0).$$

Then:

(1)
$$T^{-1} = (b^+ - b^-)^{-\frac{1}{2}}(0) \begin{pmatrix} -b^-(0) & \mathbb{1} \\ -b^+(0) & \mathbb{1} \end{pmatrix}.$$

(2)
$$T^* q T = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}.$$

(3) *Let*
$$\pi^+ = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}, \quad \pi^- = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix}$$
and
$$c^\pm := T\pi^\pm T^{-1} = \begin{pmatrix} \mp(b^+ - b^-)^{-1} b^\mp & \pm(b^+ - b^-)^{-1} \\ \mp b^+(b^+ - b^-)^{-1} b^- & \pm b^\pm (b^+ - b^-)^{-1} \end{pmatrix}(0);$$
then
$$c^+ + c^- = \mathbb{1}, \quad (c^\pm)^2 = c^\pm, \quad \operatorname{Ker} u^\mp = \operatorname{Ran} c^\pm,$$
$$(c^\mp)^* q c^\pm = 0, \quad \pm (c^\pm)^* q c^\pm \geq 0,$$
on $H^\infty(\Sigma;\mathbb{C}^2)$.

(4)
$$\mathrm{WF}(U_0 c^\pm)' \subset \mathcal{N}^\pm \times (T^*\Sigma \setminus o).$$

(5) *The map* $T : L^2(\Sigma) \oplus L^2(\Sigma) \to H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$ *is an isomorphism.*

Proof. The proof of (1) and (2) is a routine computation, and (3) follows from (2). Note that $c^\pm$ are bounded on $H^\infty(\Sigma;\mathbb{C}^2)$ and $H^{-\infty}(\Sigma;\mathbb{C}^2)$, since their entries belong to $\Psi^\infty_{\mathrm{b}}(\Sigma)$.

We have $U_0 c^\pm = \tilde{U}_0 c^\pm$ modulo $C^\infty(M \times M)$ and $\tilde{U}_0 c^\pm = \mathcal{U}^\pm(\cdot)c^\pm$ by (3), so $\mathrm{WF}(U_0 c^\pm)' = \mathrm{WF}(\mathcal{U}^+(\cdot)c^\pm)'$. By (11.10), we have $P\mathcal{U}^\pm(\cdot)c^\pm \in C^\infty(M \times M)$ hence $\mathrm{WF}(\mathcal{U}^+(\cdot)c^\pm)' \subset \mathcal{N} \times (T^*\Sigma \setminus o)$. Furthermore, $(\partial_t - \mathrm{i}b^\pm(t)\mathcal{U}^+(\cdot)c^\pm = 0$, but $\partial_t - \mathrm{i}b^\pm(t)$ is not a classical pseudodifferential operator on M. However, one can find $\chi^\pm \in \Psi^0_{\mathrm{c}}(M)$, elliptic near $\mathcal{N}^\pm$, such that $\chi^\pm \circ (\partial_t - \mathrm{i}b^\pm(t))$ belongs to $\Psi^1(M)$. We have $\chi^\pm \circ (\partial_t - \mathrm{i}b^\pm(t))\mathcal{U}^+(\cdot)c^\pm = 0$ and $\chi^\pm \circ (\partial_t - \mathrm{i}b^\pm(t))$ is elliptic near $\mathcal{N}^\mp$. Now applying Theorem 7.3.1 we conclude that $\mathrm{WF}(\mathcal{U}^+(\cdot)c^\pm)' \subset \mathcal{N}^\pm \times (T^*\Sigma \setminus o)$, which proves (4).

It remains to prove (5). Using the expression of T^{-1} in (2), we see that the norm $\|T^{-1}f\|_{L^2(\Sigma;\mathbb{C}^2)}$ is equivalent to the norm $\|(b^+ - b^-)^{\frac{1}{2}} f_0\|_{L^2(\Sigma)} + \|(b^+ - b^-)^{-\frac{1}{2}} f_1\|_{L^2(\Sigma;\mathbb{C}^2)}$. By (11.14), we have

$$c^{-1}\epsilon(0) \leq b^+(0) - b^-(0) \leq c\epsilon(0),$$

which by the Kato-Heinz theorem implies that $\|T^{-1}f\|_{L^2(\Sigma;\mathbb{C}^2)}$ is equivalent to $\|\epsilon(0)^{\frac{1}{2}} f_0\|_{L^2(\Sigma)} + \|\epsilon(0)^{-\frac{1}{2}} f_1\|_{L^2(\Sigma)}$. By the ellipticity of $\epsilon(0)$, this norm is equivalent to the norm of $H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$. □

REMARK 11.3.3. *$c^\pm$ are complementary projections, with* $\operatorname{Ran} c^\pm = \operatorname{Ker} u^\mp$. *Moreover,* $\operatorname{Ran} c^\pm$ *are orthogonal for q, with* $\mathrm{WF} U_0 c^\pm f \subset \mathcal{N}^\pm$ *for* $f \in H^{-\infty}(\Sigma)$. *Therefore the pair of projections $c^\pm$ will be called a* microlocal splitting *of Cauchy data.*

The space $H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$ *is the* charge space*, which appears in the quantization of Klein-Gordon equations. It is more natural in this context than the* energy space $H^1(\Sigma) \oplus L^2(\Sigma)$*, which is usually considered in the* PDE *literature.*

11.4. The pure Hadamard state associated to a microlocal splitting

It is now straightforward to associate a pure Hadamard state to the pair of projections $c^\pm$ in Proposition 11.3.2.

THEOREM 11.4.1. *Let $c^\pm$ be a microlocal splitting and*

$$\lambda_0^\pm := \pm q c^\pm. \tag{11.17}$$

Then $\lambda_0^\pm$ are the Σ_0 covariances of a pure Hadamard state ω_b for P.

Proof. We first check the conditions in Proposition 6.1.5. (i) is obvious and (iii) follows from $c^+ + c^- = 1$. To check (ii), we note that $c^\pm : C_0^\infty(\Sigma; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^2)$ since $c^\pm : H^\infty(\Sigma; \mathbb{C}^2) \to H^\infty(\Sigma; \mathbb{C}^2)$. We have then

$$\big(f | \lambda_0^\pm f\big)_0 = \pm \big((c^+ + c^-) f | q c^\pm f\big)_0 = \pm \big(c^\pm f | q c^\pm f\big)_0 \geq 0,$$

by Proposition 11.3.2 (3). Therefore $\lambda_0^\pm$ are the Σ_0 covariances of a quasi-free state ω_b for P.

If $\Lambda^\pm$ are the spacetime covariances of ω_b, we deduce from Proposition 11.1.1 and Proposition 11.3.2 (4) that $\mathrm{WF}(\Lambda^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}$. Since $(\Lambda^\pm)^* = \Lambda^\pm$ we have $\mathrm{WF}(\Lambda^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm$, hence by Theorem 8.4.2 ω_b is a Hadamard state.

It remains to prove that ω_b is pure. To that end, let us first examine the norm $\| \cdot \|_\omega$ associated to ω_b, see Subsection 4.9.2. By Proposition 11.3.2, we have

$$\lambda_0^+ + \lambda_0^- = qT(\pi^+ - \pi^-)T^{-1} = (T^{-1})^*(\pi^+ - \pi^-)^2 T^{-1} = (T^{-1})^* T^{-1}.$$

Therefore, $\|f\|_\omega^2 = (f | (\lambda^+ + \lambda^-) f)_{L^2(\Sigma; \mathbb{C}^2)} = \|T^{-1} f\|^2_{L^2(\Sigma; \mathbb{C}^2)}$. By Proposition 11.3.2 (5), the completion $\mathcal{Y}^{\mathrm{cpl}}$ of $\mathcal{Y} = C_0^\infty(\Sigma; \mathbb{C}^2)$ with respect to the norm $\| \cdot \|_\omega$ equals $H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$.

Again by Proposition 11.3.2 (5), we obtain that $c^\pm = T \pi^\pm T^{-1}$ extend by density to projections on $\mathcal{Y}^{\mathrm{cpl}}$ that satisfy (4.36) in Proposition 4.9.3. Therefore, ω_b is a pure state. □

11.5. Spacetime covariances and Feynman inverses

We now give more explicit formulas expressing the spacetime covariances $\Lambda^\pm$ of ω_b and the Feynman inverse associated to ω_b, see Section 8.5.

It is convenient to formulate these results using the 'time kernel' notation: namely, if $A : C_0^\infty(M; \mathbb{C}^p) \to C^\infty(M; \mathbb{C}^q)$ we denote by $A(t,s) : C_0^\infty(\Sigma; \mathbb{C}^p) \to C^\infty(\Sigma; \mathbb{C}^q)$ its operator-valued kernel, defined by

$$Au(t) = \int_{\mathbb{R}} A(t,s) u(s) ds, \quad u \in C_0^\infty(M; \mathbb{C}^p).$$

If $\mathcal{U}_H(t,s)$ is the propagator introduced in (11.5), we set

$$\mathcal{U}_H^\pm(t,s) := \mathcal{U}_H(t,0) c^\pm \mathcal{U}_H(0,s).$$

The following theorem is shown in [**GOW**, Theorems 6.8, 7.10].

THEOREM 11.5.1. *Let $\Lambda^\pm$ and $G_{\rm F}$ be the spacetime covariances and the Feynman inverse, respectively, of the state ω_b constructed in Theorem* 11.4.1. *Then*

$$\begin{aligned}\Lambda^\pm(t,s) &= \pm\pi_0\mathcal{U}_H^\pm(t,s)\pi_1^*,\\ G_{\rm F}(t,s) &= \mathrm{i}^{-1}\pi_0\left(\mathcal{U}_H^+(t,s)\theta(t-s)-\mathcal{U}_H^-(t,s)\theta(s-t)\right)\pi_1^*,\end{aligned}\tag{11.18}$$

where $\pi_i\begin{pmatrix} f_0\\ f_1\end{pmatrix}=f_i$ and $\theta(t)$ is the Heaviside function.

Let us conclude this subsection by stating without proofs some more results taken from [**GOW**, Section 7].

11.5.1. Regular states. Recall that $\Sigma_s=\{s\}\times\Sigma$ for $s\in I$ and let $\lambda_s^\pm$ be the Cauchy surface covariances of ω_b on Σ_s. Then one can show that

$$\lambda_s^\pm=\pm qc^\pm(s),$$

where $c^\pm(s)=T(s)\pi^\pm T^{-1}(s)$ and $T(s)$ is defined as in Proposition 11.3.2, with $b^\pm(0)$ replaced by $b^\pm(s)$.

A quasi-free state ω for P is called *regular* if its Cauchy surface covariances $\lambda_s^\pm$ on Σ_s belong to $\Psi_{\rm b}^\infty(\Sigma;M_2(\mathbb{C}))$ for *some* $s\in I$. One can show that if ω is regular, then $\lambda_s^\pm$ on $\Sigma_s\in\Psi_{\rm b}^\infty(\Sigma;M_2(\mathbb{C}))$ for *all* $s\in I$.

11.5.2. Bogoliubov transformations. It is well known, see e.g. [**DG**, Theorem 11.20] that if $(\mathcal{Y},q)$ is a Hermitian space and if $\omega,\tilde\omega$ are two pure quasi-free states on $\mathrm{CCR}^{\rm pol}(\mathcal{Y},q)$, then there exists $u\in U(\mathcal{Y},q)$ such that

$$\tilde\lambda^\pm=u^*\lambda^\pm u.$$

Such a map u corresponds to a *Bogoliubov transformation*.

One can show that if ω is a pure, regular Hadamard state for P, with covariances $\lambda_0^\pm$ on Σ_0, then there exists $a\in\mathcal{W}^{-\infty}(\Sigma)$ such that

$$\lambda_0^\pm=\pm T^{-1}(0)^*U^*\pi^\pm UT^{-1}(0),\ \text{ with } U=\begin{pmatrix}(\mathbb{1}+aa^*)^{\frac12} & a\\ a^* & (\mathbb{1}+a^*a)^{\frac12}\end{pmatrix}.$$

11.6. Klein-Gordon operators on Lorentzian manifolds of bounded geometry

We now introduce a class of spacetimes and associated Klein-Gordon equations whose analysis can be reduced to the model situation in Section 11.2. The results in this subsection are taken from [**GOW**, Section 3]. We start with some definitions.

11.6.1. Lorentzian manifolds of bounded geometry. Let M a smooth manifold equipped with a reference Riemannian metric $\hat h$ such that $(M,\hat h)$ is of bounded geometry.

DEFINITION 11.6.1. *If g is a Lorentzian metric on M, we say that (M,g) is of* bounded geometry *if $g\in BT_2^0(M,\hat h)$ and $g^{-1}\in BT_0^2(M,\hat h)$.*

DEFINITION 11.6.2. *Let Σ an $(n-1)$-dimensional submanifold. An embedding $i:\Sigma\to M$ is called* of bounded geometry *if there exists a family $\{U_x,\psi_x\}_{x\in M}$ of bounded chart diffeomorphisms for $\hat h$ such that if $\Sigma_x:=\psi_x(i(\Sigma)\cap U_x)$ we have*

$$\Sigma_x=\{(v',v_n)\in B_n(0,1):\ v_n=F_x(v')\},$$

where $\{F_x\}_{x\in M}$ is a bounded family in $C_{\rm b}^\infty(B_{n-1}(0,1))$.

The typical example of an embedding of bounded geometry is as follows: let $M = I \times S$, where I is an open interval and (S, h) is of bounded geometry, and let $\hat{h} = dt^2 + h(x)dx^2$. Then the submanifolds $\{t = F(x)\}$ for $F \in BT_0^0(S, h)$ are of bounded geometry in $(M, \hat{h})$.

DEFINITION 11.6.3. *A space-like Cauchy surface $\Sigma \subset M$ is of* bounded geometry *if:*

(1) *the injection $i : \Sigma \to M$ is of bounded geometry for $\hat{h}$;*
(2) *if $n(y)$ for $y \in \Sigma$ is the future directed unit normal to Σ for g, then*

$$\sup_{y\in\Sigma} n(y) \cdot \hat{h}(y)n(y) < \infty.$$

Clearly, the above definitions depend only on the equivalence class of $\hat{h}$ for the equivalence relation $\sim$ in Subsection 10.3.5.

11.6.2. Gaussian normal coordinates. The following result is proved in [**GOW**, Theorem 3.5]. It says that the bounded geometry property of g and Σ carries over to the Gaussian normal coordinates to Σ.

THEOREM 11.6.4. *Let (M, g) a Lorentzian manifold of bounded geometry and Σ a Cauchy surface of bounded geometry. Then the following holds:*

(1) *there exists $\delta > 0$ such that the normal geodesic flow to Σ:*

$$\chi : \begin{array}{l}]-\delta, \delta[\times\Sigma \longrightarrow M \\ (t, y) \longmapsto \exp_y^g(tn(y)) \end{array}$$

is well defined and is a smooth diffeomorphism onto its range;

(2) *$\chi^* g = -dt^2 + h_t$, where $\{h_t\}_{t\in]-\delta,\delta[}$ is a smooth family of Riemannian metrics on Σ such that*

(i) *(Σ, h_0) is of bounded geometry,*
(ii) *$t \mapsto h_t \in C_{\mathrm{b}}^\infty(\,]-\delta, \delta[, BT_2^0(\Sigma, h_0))$,*
(iii) *$t \mapsto h_t^{-1} \in C_{\mathrm{b}}^\infty(\,]-\delta, \delta[, BT_0^2(\Sigma, h_0))$.*

11.6.3. Klein-Gordon operators on Lorentzian manifolds of bounded geometry. Let (M, g) a globally hyperbolic spacetime of bounded geometry, with respect to a reference Riemannian metric $\hat{h}$. We fix a 1-form $A_\mu dx^\mu \in BT_1^0(M, \hat{h})$ and a real function $V \in BT_0^0(M, \hat{h})$, and consider the associated Klein-Gordon operator P as in Subsection 5.5.1. Note that $P \in \mathrm{Diff}_{\mathrm{b}}^2(M, \hat{h})$.

Let $\chi :]-\delta, \delta[\times\Sigma \to M$ the diffeomorphism in Theorem 11.6.4 and let us still denote by $A_\mu dx^\mu$, V and P their respective pullbacks by χ. Then P equals

$$P = |h_t|^{-\frac{1}{2}}(\partial_t - \mathrm{i}qA_0)|h_t|^{\frac{1}{2}}(\partial_t - \mathrm{i}qA_0) - |h_t|^{-\frac{1}{2}}(\partial_j - \mathrm{i}qA_j)|h_t|^{\frac{1}{2}}h_t^{jk}(\partial_k - \mathrm{i}qA_k) + V.$$

Setting $F(t, x) = q\int_0^t A_0(s, x)dx$, we have $\mathrm{e}^{-\mathrm{i}F}(\partial_t - \mathrm{i}qA_0)\mathrm{e}^{\mathrm{i}F} = \partial_t$, hence

$$P_{\mathrm{red}} = \mathrm{e}^{-\mathrm{i}F} P \mathrm{e}^{\mathrm{i}F}$$

is a model Klein-Gordon operator of the form (11.2).

If $\Lambda_{\mathrm{red}}^\pm$ are the spacetime covariances of the pure Hadamard state for P_{red} constructed in Theorem 11.4.1, then $\Lambda^\pm = \mathrm{e}^{\mathrm{i}F}\Lambda_{\mathrm{red}}^\pm \mathrm{e}^{-\mathrm{i}F}$ are the covariances of a pure Hadamard state for P, on $]-\delta, \delta[\times\Sigma$. Pushing $\Lambda^\pm$ to M by χ, we obtain a pure Hadamard state for the original Klein-Gordon operator on M.

11.7. Conformal transformations

The conditions in Section 11.6 are rather strong, since they imply in particular that (M, g) has a Cauchy surface Σ such that the normal geodesic flow to Σ exists for some uniform time interval. However it is possible to greatly enlarge the class of Klein-Gordon equations which can reduced to the model case in Section 11.2.

Thus, let

$$P = -(\nabla^\mu - \mathrm{i}qA^\mu(x))(\nabla_\mu - \mathrm{i}qA_\mu(x)) + V(x)$$

be a Klein-Gordon operator on (M, g), Σ be a space-like Cauchy surface for (M, g) and $\hat{h}$ be a reference Riemannian metric on M such that $(M, \hat{h})$ is of bounded geometry.

As in Section 6.3, we consider $\tilde{g} = c^2 g$ and $\tilde{P} = c^{-n/2-1} P c^{n/2-1}$.

One can check that if

(i) $(M, \tilde{g})$ is of bounded geometry for $\hat{h}$,

(ii) Σ is of bounded geometry in $(M, \tilde{g})$,

(iii) $c^{-2}V \in BT^0_0(M, \hat{h})$, $A_\mu dx^\mu, c^{-1}\nabla_\mu c dx^\mu \in BT^0_1(M, \hat{h})$,

then $\tilde{P}$ is Klein-Gordon operator on $(M, \tilde{g})$ belonging to $\mathrm{Diff}_{\mathrm{b}}(M, \hat{h})$. Therefore, $\tilde{P}$ can be reduced to the model case, over a causally compatible neighborhood of Σ in M. The pure Hadamard state for $\tilde{P}$ constructed as in Section 11.4 yields by Section 8.6 a pure Hadamard state for P.

11.7.1. Examples. As mentioned in the introduction, the above reduction can be applied for example to the Kerr or Kerr-de Sitter exterior spacetimes and the Kerr-Kruskal spacetime for $A_\mu = 0$, $V = m^2$. Other examples are cones, double cones and wedges in Minkowski spacetime. We refer the reader to [**GOW**, Section 4] for details.

11.8. Hadamard states on general spacetimes

Let us now go back to the general situation, where (M, g) is a globally hyperbolic spacetime and P a Klein-Gordon operator on (M, g). Let us fix a space-like Cauchy surface Σ in (M, g). We will prove the following theorem, which follows from a construction in [**GW1**, Section 8.2]. The classes $\Psi^\infty_{(\mathrm{c})}(\Sigma)$ were introduced in Section 10.2.

THEOREM 11.8.1. *Let P a Klein-Gordon operator on the globally hyperbolic spacetime (M, g) and Σ a space-like Cauchy surface Σ in (M, g). Then:*

(1) *there exists a Hadamard state ω for P whose Cauchy surface covariances $\lambda^\pm_\Sigma$ belong to $\Psi^\infty_{\mathrm{c}}(\Sigma; M_2(\mathbb{C}))$;*

(2) *the Cauchy surface covariances $\lambda^\pm_\Sigma$ of* any *Hadamard state ω for P belong to $\Psi^\infty(\Sigma; M_2(\mathbb{C}))$.*

Proof. Let us first note that (2) follows from (1). Indeed, let ω_1 be the Hadamard state in (1) and let ω be another Hadamard state. By Corollary 8.4.3, $\Lambda^\pm - \Lambda^\pm_1$ have smooth kernels, hence $\lambda^\pm_\Sigma - \lambda^\pm_{\Sigma,1}$ have smooth kernels by Proposition 6.1.6 (2). Since $\lambda^\pm_{\Sigma,1} \in \Psi^\infty_{\mathrm{c}}(\Sigma; M_2(\mathbb{C}))$, we see that $\lambda^\pm_\Sigma \in \Psi^\infty(\Sigma; M_2(\mathbb{C}))$.

It remains to prove (1). By Proposition 5.4.7, we can assume that M is a neighborhood U of $\{0\} \times \Sigma$ in $\mathbb{R} \times \Sigma$ and $g = -dt^2 + h_t(x)dx^2$. Let us fix an atlas $\{V_i, \psi_i\}_{i\in\mathbb{N}}$ of Σ with V_i relatively compact and relatively compact open intervals I_i, $i \in \mathbb{N}$ with $0 \in I_i$ and $I_i \times V_i \Subset U$.

The metrics $(\psi_i^{-1})^* h_t$ can be extended to metrics $\tilde{h}_{it}$ on $\mathbb{R}^d$ such that $\tilde{h}_{it} \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^0_2(\mathbb{R}^d))$ and $\tilde{h}^{-1}_{it} \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^2_0(\mathbb{R}^d))$, where we equip $\mathbb{R}^d$ with the flat metric δ. This means that for each $i \in \mathbb{N}$ the derivatives in (t, x) of $\tilde{h}_{it}$ and $\tilde{h}^{-1}_{it}$

are uniformly bounded on $\mathbb{R}\times\mathbb{R}^d$. The Klein-Gordon operators $\psi_i\circ P\circ\psi_i^{-1}$ can similarly be extended as Klein-Gordon operators $\tilde{P}_i$ on $\mathbb{R}\times\mathbb{R}^d$ which belong to $\mathrm{Diff}_{\mathrm{b}}(\mathbb{R}^{1+d})$.

We fix a partition of unity $1=\sum_{i\in\mathbb{N}}\chi_i^2$ subordinate to the cover $\{V_i\}_{i\in\mathbb{N}}$. Note that if $q=\begin{pmatrix}0&\mathbb{1}\\ \mathbb{1}&0\end{pmatrix}$, then in view of the expression (5.31) of q_Σ we have

$$q_\Sigma=\sum_{i\in\mathbb{N}}\chi_i\psi_i^*(q)\chi_i. \tag{11.19}$$

Let $\tilde{\lambda}_i^\pm$ be the Cauchy surface covariances in Theorem 11.4.1 for $\tilde{P}_i$ and the Cauchy surface $\{t=0\}$ in $\mathbb{R}\times\mathbb{R}^d$. We set

$$\lambda^\pm:=\sum_{i\in\mathbb{N}}\chi_i\psi_i^*(\tilde{\lambda}_i^\pm)\chi_i.$$

By (11.19), we have $\lambda_\Sigma^+-\lambda_\Sigma^-=q_\Sigma$. Moreover, $\lambda_\Sigma^\pm\geq 0$, since $\tilde{\lambda}_i^\pm\geq 0$. Let ω_U be the associated quasi-free state for P on (U,g). By Proposition 11.1.1 and the covariance of the wavefront set under diffeomorphisms, we obtain that ω_U is a Hadamard state for P on (U,g).

Now we apply the time-slice property Proposition 5.6.4 and the propagation of singularity theorem to extend ω_U to a Hadamard state ω for P on (M,g). Its Cauchy surface covariances on Σ are of course equal to $\lambda_\Sigma^\pm$. Since $\tilde{\lambda}_i^\pm\in\Psi_{\mathrm{b}}^\infty(\mathbb{R}^d;M_2(\mathbb{C}))$, we obtain that $\lambda_\Sigma^\pm\in\Psi_{\mathrm{c}}^\infty(\Sigma;M_2(\mathbb{C}))$, by the definition of $\Psi_{\mathrm{c}}^\infty(\Sigma)$. This completes the proof of (1). □

CHAPTER 12

Analytic Hadamard states and Wick rotation

In Minkowski spacetime the *Wick rotation* consists in the substitution $t \mapsto \mathrm{i}s$. The Minkowski space $\mathbb{R}^{1,d}$ becomes the Euclidean space $\mathbb{R}^{1+d}$ and the wave operator $-\Box$ becomes the *Laplacian* $-\Delta$.

Being elliptic, the operator $-\Delta + m^2$ has a unique inverse G_{E}, given by

$$G_{\mathrm{E}} v(s,\cdot) = \int_{\mathbb{R}} G_{\mathrm{E}}(s-s')v(s',\cdot)ds',$$

with

$$G_{\mathrm{E}}(s) = (2\epsilon)^{-1}(\mathrm{e}^{-s\epsilon}\theta(s) + \mathrm{e}^{s\epsilon}\theta(-s)),$$

where we recall that $\epsilon = (-\Delta_{\mathrm{x}} + m^2)^{\frac{1}{2}}$. A remarkable fact is that

$$\mathrm{i}^{-1} G_{\mathrm{E}}(\mathrm{i}t) = G_{\mathrm{F}}(t),$$

where, see (8.20), $G_{\mathrm{F}}(t)$ is the kernel of the Feynman inverse associated to the *vacuum state* for $-\Box + m^2$. The Wick rotation or Euclidean approach is particularly important when one tries to construct *interacting* field theories. It is the basis of the *constructive field theory*, whose most celebrated achievements are the rigorous constructions of the $P(\varphi)_2$ and φ^4_3 theories. We refer the reader to the books of Glimm and Jaffe [**GJ**] and Simon [**Si**], or to [**DG**, Chap. 21], for a detailed exposition.

In the Euclidean approach the main goal is the construction of an 'interacting' probability measure on a path space, or the construction of its moments, which are called *Schwinger functions*. The return to the Lorentzian world can be done by 'reconstruction theorems', like the Osterwalder-Schrader theorem. This step is actually often forgotten, to such an extent that physicists speaking of quantum field theories often have in mind their Euclidean versions.

It is clear that the Wick rotation can be defined if we replace $\mathbb{R}^{1,d}$ by an ultra-static spacetime, see Section 5.3, if we set $\epsilon = (-\Delta_h + m^2)^{\frac{1}{2}}$. Static spacetimes are reduced to ultra-static ones by the procedure explained in Section 9.4 and with some more effort stationary spacetimes can be treated as well, see [**G2**].

For general spacetimes, its not clear what the Wick rotation should mean, since there is no canonical time coordinate. In this chapter we will explain a result of [**GW5**], where the Wick rotation is performed in the Gaussian time coordinate near a Cauchy surface of (M, g). To the elliptic operator obtained by Wick rotation one can associate the so-called *Calderón projectors*, which are a standard tool in elliptic boundary value problems.

It turns out that it is possible to use the Calderón projectors to define a pure quasi-free state for a Klein-Gordon operator on (M, g). This state has the important property of being an *analytic Hadamard state*. As a consequence, it satisfies the *Reeh-Schlieder* property.

12.1. Boundary values of holomorphic functions

Let us recall the well-known definition of distributions as boundary values of holomorphic functions.

12.1.1. Notation. We first introduce some notation.

- A cone of vertex 0 in $\mathbb{R}^n$, which is convex open and proper, will be simply called a *convex open cone*. If Γ, Γ' are two cones of vertex 0 in $\mathbb{R}^n$ we write $\Gamma' \Subset \Gamma$ if $(\Gamma' \cap \mathbb{S}^{n-1}) \Subset (\Gamma \cap \mathbb{S}^{n-1})$.

- We recall that Γ° denotes the polar of Γ, see (8.16). Γ° is a closed convex cone.

- Let $\Omega \subset \mathbb{R}^n$ be open and let $\Gamma \subset \mathbb{R}^n$ be a convex open cone. Then a domain $D \subset \mathbb{C}^n$ is called a *tuboid of profile* $\Omega + \mathrm{i}\Gamma$ if

(1) $D \subset \Omega + \mathrm{i}\Gamma$,

(2) for any $x_0 \in \Omega$ and any subcone $\Gamma' \Subset \Gamma$ there exists a neighborhood Ω' of x_0 in Ω and $r > 0$ such that

$$\Omega' + \mathrm{i}\{y \in \Gamma' : 0 < |y| \leq r\} \subset D.$$

- If $D \subset \mathbb{C}^n$ is open, we denote by $\mathscr{O}(D)$ the space of holomorphic functions in D.

- We write $F \in \mathscr{O}_{\mathrm{temp}}(\Omega + \mathrm{i}\Gamma 0)$ and say that F is *temperate*, if $F \in \mathscr{O}(D)$ for some tuboid D of profile $\Omega + \mathrm{i}\Gamma$ and if for any $K \Subset \Omega$, any subcone $\Gamma' \Subset \Gamma$, there exist $C, r > 0$ and $N \in \mathbb{N}$ such that $K + \mathrm{i}\{y \in \Gamma' : 0 < |y| \leq r\} \subset D$ and

$$|F(x + \mathrm{i}y)| \leq C|y|^{-N}, \quad x \in K, \ y \in \Gamma', \ 0 < |y| \leq r. \tag{12.1}$$

12.1.2. Boundary values of holomorphic functions. If $F \in \mathscr{O}_{\mathrm{temp}}(\Omega + \mathrm{i}\Gamma 0)$ the limit

$$\lim_{\Gamma' \ni y \to 0} F(x + \mathrm{i}y) = f(x) \ \text{ exists in } \mathcal{D}'(\Omega), \tag{12.2}$$

for any $\Gamma' \Subset \Gamma$ and is denoted by $F(x + \mathrm{i}\Gamma 0)$, (see e.g. [**Ko**, Theorem 3.6]).

If $\Gamma_1, \ldots, \Gamma_N$ are convex open cones such that $\bigcup_1^N \Gamma_i^\circ = \mathbb{R}^n$, then any $u \in \mathcal{D}'(\Omega)$ can be written as

$$u(x) = \sum_{j=1}^N F_j(x + \mathrm{i}\Gamma_j 0), \tag{12.3}$$

for some $F_j \in \mathscr{O}_{\mathrm{temp}}(\Omega + \mathrm{i}\Gamma_j 0)$. This fact comes from the construction of a so-called *decomposition of* δ, see e.g. [**H1**, Theorem 8.4.11]. If $n = 1$ this is simply the identity $\delta(x) = (2\mathrm{i}\pi)^{-1}((x + \mathrm{i}0)^{-1} - (x - \mathrm{i}0)^{-1})$.

The non-uniqueness of the decomposition (12.3) is described by *Martineau's edge of the wedge theorem*, which states that

$$\sum_{j=1}^N F_j(x + \mathrm{i}\Gamma_j 0) = 0 \quad \text{in } \mathcal{D}'(\Omega)$$

for $F_j \in \mathscr{O}_{\mathrm{temp}}(\Omega + \mathrm{i}\Gamma_j 0)$ iff there exist $H_{jk} \in \mathscr{O}_{\mathrm{temp}}(\Omega + \mathrm{i}\Gamma_{jk} 0)$, with $\Gamma_{jk} = (\Gamma_j + \Gamma_k)^{\mathrm{conv}}$ (A^{conv} denotes the convex hull of A) such that

$$F_j = \sum_k H_{jk} \text{ in } \Omega + \mathrm{i}\Gamma_j, \quad H_{jk} = -H_{kj} \text{ in } \Gamma_{jk},$$

see for example [**Ko**, Theorem 3.9].

12.1.3. Partial boundary values. One can also obtain distributions as boundary values of partially holomorphic distributions in one variable, as in Proposition 7.1.5. Let us assume that $\Omega = I \times Y$, where $I \subset \mathbb{R}$ is an open interval and $Y \subset \mathbb{R}^{n-1}$ is open, writing $x \in \Omega$ as (t, y).

We denote by $\mathscr{O}_{\mathrm{temp}}(I \pm \mathrm{i}0; \mathcal{D}'(Y))$ the space of temperate $\mathcal{D}'(Y)$-valued holomorphic functions on some tuboid D of profile $I \pm \mathrm{i}0$. This means that for each

$K \Subset I$ there exist $r > 0$ and $N \in \mathbb{N}$, such that for each bounded set $B \subset \mathcal{D}(Y)$ there exist $C_B > 0$ such that

$$\sup_{\varphi \in B} |\langle u(z,\cdot), \varphi(\cdot)\rangle_Y| \leq C_B |\mathrm{Im}\, z|^{-N}, \quad \mathrm{Re}\, z \in K, \ \pm \mathrm{Im}\, z > 0, \ |\mathrm{Im}\, z| \leq r,$$

where $\langle \cdot, \cdot \rangle_Y$ is the duality bracket between $\mathcal{D}'(Y)$ and $\mathcal{D}(Y)$.

Let us set $\varphi_z(s) = (s-z)^{-1}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. If $u \in \mathcal{D}'(\mathbb{R} \times \mathbb{R}^{n-1})$ has compact support, then

$$F(z,y) = \frac{1}{2\mathrm{i}\pi} \langle \varphi_z(\cdot), F(\cdot, y)\rangle_{\mathbb{R}}$$

belongs to $\mathscr{O}_{\mathrm{temp}}(\mathbb{R} \pm \mathrm{i}0; \mathcal{D}'(\mathbb{R}^{n-1}))$ and

$$u(s,y) = F(s + \mathrm{i}0, y) - F(s - \mathrm{i}0, y),$$

where $F(s \pm \mathrm{i}0, y) = \lim_{\epsilon \to 0^\pm} F(s + \mathrm{i}\epsilon, y)$ in $\mathcal{D}'(\mathbb{R} \times \mathbb{R}^{n-1})$.

12.2. The analytic wavefront set

We now recall the definition of the *analytic wavefront set* of a distribution on $\mathbb{R}^n$ originally due to Bros and Iagolnitzer [**BI**], following [**Sj**]. We set

$$\varphi_z^\lambda(x) := \mathrm{e}^{-\frac{\lambda}{2}(z-x)^2}, \quad z \in \mathbb{C}^n, \ x \in \mathbb{R}^n, \ \lambda \geq 1.$$

Definition 12.2.1. *Let $\Omega \subset \mathbb{R}^n$ be an open set. A point $(x_0, \xi_0) \in T^*\Omega \setminus o$ does not belong to the* analytic wavefront set $\mathrm{WF}_a u$ *of $u \in \mathcal{D}'(\Omega)$ if there exist a cutoff function $\chi \in C_0^\infty(\Omega)$ with $\chi = 1$ near x_0, a neighborhood W of $x_0 - \mathrm{i}\xi_0$ in $\mathbb{C}^n$, and constants $C, \epsilon > 0$ such that*

$$|\langle u | \chi \varphi_z^\lambda \rangle| \leq C \mathrm{e}^{\frac{\lambda}{2}((\mathrm{Im} z)^2 - \epsilon)}, \quad z \in W, \ \lambda \geq 1, \tag{12.4}$$

where $\langle \cdot | \cdot \rangle$ is the duality bracket between $\mathcal{D}'(\mathbb{R}^n)$ and $C_0^\infty(\mathbb{R}^n)$.

Note that in Definition 12.2.1 one identifies $\mathbb{R}^n$ with $(\mathbb{R}^n)'$ using the quadratic form $x \cdot x$ appearing in the definition of φ_z^λ.

If $u \in \mathcal{E}'(\mathbb{R}^n)$, the holomorphic function $\mathbb{C}^n \ni z \mapsto T_\lambda u(z) = \langle u | \varphi_z^\lambda \rangle$ is called the F.B.I. *transform* of u.

The C^∞ wavefront set $\mathrm{WF}u$ can also be characterized by the F.B.I. transform, if one requires instead of (12.4) that

$$|\langle u | \chi \varphi_z^\lambda \rangle| \leq C_N \mathrm{e}^{\frac{\lambda}{2}(\mathrm{Im} z)^2} \lambda^{-N}, \quad z \in W, \ \lambda \geq 1, \ N \in \mathbb{N}, \tag{12.5}$$

see e.g. [**De**, Corollary 1.4]. The projection of $\mathrm{WF}_a u$ on $\mathbb{R}^n$ is equal to the *analytic singular support* $\mathrm{singsupp}_a u$.

The analytic wavefront set is covariant under analytic diffeomorphisms, which allows to extend its definition to distributions on a real analytic manifold M in the usual way.

There is an equivalent definition of $\mathrm{WF}_a u$ based on the representation of a distribution as sum of boundary values of temperate holomorphic functions. The equivalence of the two definitions was shown by Bony [**Bo**], who also showed the equivalence with a third definition due to Hörmander, see [**H1**, Definition 8.4.3].

Definition 12.2.2. *Let $u \in \mathcal{D}'(\Omega)$ for $\Omega \subset \mathbb{R}^n$ open and $(x^0, \xi^0) \in \Omega \times \mathbb{R}^n \setminus \{0\}$. Then (x^0, ξ^0) does not belong to $\mathrm{WF}_a u$ if there exist $N \in \mathbb{N}$, a neighborhood Ω' of x^0 in Ω, and convex open cones Γ_j, $1 \leq j \leq N$, such that*

$$u(x) = \sum_{j=1}^N F_j(x + \mathrm{i}\Gamma_j 0) \text{ over } \Omega',$$

for $F_j \in \mathscr{O}_{\mathrm{temp}}(\Omega' + \mathrm{i}\Gamma_j 0)$, $1 \leq j \leq N$, and F_j holomorphic near x^0 if $\xi^0 \in \Gamma_j^\circ$.

Theorem 7.3.1 extends to the analytic wavefront set, at least when one considers differential operators. For completeness let us state this extension, see (see [**Kw**, Theorem 3.3'] or [**H5**, Theorems 5.1, 7.1]).

THEOREM 12.2.3. *Let X be a real analytic manifold and $P \in \mathrm{Diff}^m(X)$ be an analytic differential operator of order m. Then for $u \in \mathcal{D}'(X)$ we have*

(1) $\mathrm{WF}_a(u) \setminus \mathrm{WF}_a(Pu) \subset \mathrm{Char}(P)$ (microlocal ellipticity),

(2) *If P is of real principal type with $\partial_\xi p_m(x,\xi) \neq 0$ on $\mathrm{Char}(P)$, then $\mathrm{WF}_a(u) \setminus \mathrm{WF}_a(Pu)$ is invariant under the flow of H_p* (propagation of singularities).

The analytic wavefront set of a distribution has deep relations with its support. An example of such a relation is the *Kashiwara-Kawai theorem*, which we now explain.

If $F \subset M$ is a closed set, the *normal set* $N(F) \subset T^*M \setminus o$ is the set of (x^0, ξ^0) such that $x^0 \in F$, $\xi^0 \neq 0$, and there exists a real function $f \in C^2(M)$ such that $df(x^0) = \xi^0$ or $df(x^0) = -\xi^0$ and $F \subset \{x : f(x) \leq f(x^0)\}$. Note that $N(F) \subset T^*_{\partial F} M$ and $N(F) = N^*(\partial F)$ if ∂F is a smooth hypersurface.

The *Kashiwara-Kawai theorem* (see e.g. [**H2**, Theorem 8.5.6']) states that

$$N(\operatorname{supp} u) \subset \mathrm{WF}_a(u), \quad \forall\, u \in \mathcal{D}'(M). \tag{12.6}$$

We end this subsection by stating the analog of Proposition 7.1.5 for the analytic wavefront set, which is proved in [**K**, Theorem 4.3.10].

PROPOSITION 12.2.4. *Let $F \in \mathscr{O}_{\mathrm{temp}}(I \pm \mathrm{i}0; \mathcal{D}'(Y))$. Then*

$$\mathrm{WF}_a(F(t \pm \mathrm{i}0, y)) \subset \{\tau \geq 0\}.$$

12.3. Analytic Hadamard states

A spacetime (M, g) is called *analytic* if M is a real analytic manifold and g is an analytic Lorentzian metric on M. Similarly, a Klein-Gordon operator P as in Subsection 5.5.1 is *analytic* if (M, g) and $A_\mu dx^\mu, V$ are analytic.

In [**SVW**] Strohmaier, Verch and Wollenberg introduced the notion of *analytic Hadamard states*, obtained from Definition 8.3.2 by replacing the C^∞ wavefront set WF by the *analytic wavefront set* WF_a.

DEFINITION 12.3.1. *A quasi-free state for P is an* analytic Hadamard state if its spacetime covariances $\Lambda^\pm$ satisfy

$$\mathrm{WF}_a(\Lambda^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm. \tag{12.7}$$

Note that in [**SVW**] the analytic Hadamard condition is defined also for more general states for P by extending the microlocal spectrum condition of Brunetti, Fredenhagen and Köhler [**BFK**] on the n-point functions to the analytic case.

It is quite likely that the results of Section 7.4 on distinguished parametrices for Klein-Gordon operators extend to the analytic setting, although we do not know a published reference. We content ourselves with stating the extension of Corollary 8.4.3, see [**GW5**, Proposition 2.8]

PROPOSITION 12.3.2. *Let $\Lambda_i^\pm$, $i = 1, 2$ be the spacetime covariances of two analytic Hadamard states ω_i. Then $\Lambda_1^\pm - \Lambda_2^\pm$ have analytic kernels.*

Proof. Let $R^\pm = \Lambda_1^\pm - \Lambda_2^\pm$. Since $\Lambda_1^+ - \Lambda_1^- = \Lambda_2^+ - \Lambda_2^- = \mathrm{i}G$, we have $R^+ = -R^-$. On the other hand, from (12.7) we have $\mathrm{WF}_a(R^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm$, hence $\mathrm{WF}_a(R^+)' \cap \mathrm{WF}_a(R^-)' = \emptyset$. Since $R^- = -R^+$, this implies that $\mathrm{WF}_a(R^\pm)' = \emptyset$, and so $R^\pm$ have analytic kernels. □

12.4. The Reeh-Schlieder property of analytic Hadamard states

An important property of analytic Hadamard states, proved in **[SVW]**, is that they satisfy the Reeh-Schlieder property. The Reeh-Schlieder property of a state has important consequences. For example, it allows us to apply the Tomita-Takesaki modular theory to the local von Neumann algebras associated to a bounded region $O \subset M$.

We start with a lemma, related to a result of Strohmaier, Verch and Wollenberg, see **[SVW**, Propositions 2.2, 2.6**]**. Note that the notion of Hilbert space valued distributions, used in **[SVW]**, is not necessary. We first recall some notation.

If $\Lambda^\pm$ are the spacetime covariances of a Hadamard state for P, we denote by $\mathcal{Y}^{\rm cpl}$ the completion of $\mathcal{Y} = C_0^\infty(M)$ with respect to the scalar product $(f|g)_\omega = (f|\Lambda^+ g)_M + (f|\Lambda^- g)_M$. Note that $\Lambda^\pm$ extend as bounded, positive sesquilinear forms on $\mathcal{Y}^{\rm cpl}$, still denoted by $\Lambda^\pm$.

As in Section 6.2 we set for $u \in \mathcal{Y}^{\rm cpl}$

$$w_u^\pm(f) := \overline{u}\cdot\Lambda^\pm f, \quad f \in C_0^\infty(M),$$

and we recall that $w_u^\pm \in \mathcal{D}'(M)$ and

$$|w_u^\pm(f)| \leq (\overline{u}\cdot\Lambda^\pm u)^{\frac{1}{2}}(\overline{f}\cdot\Lambda^\pm f)^{\frac{1}{2}}. \tag{12.8}$$

LEMMA 12.4.1. *Let $X_0 = (x_0, \xi_0) \in T^*\mathbb{R}^n \setminus o$. Then for any $u \in \mathcal{Y}^{\rm cpl}$ one has*

$$X_0 \in \mathrm{WF}_{(a)}(w_u^\pm) \Longrightarrow (X_0, X_0) \in \mathrm{WF}_{(a)}(\Lambda^\pm)'.$$

Proof. We can assume that $M = \mathbb{R}^n$. Let $X_0 = (x_0, \xi_0) \in T^*\mathbb{R}^n \setminus o$ with $(X_0, X_0) \notin \mathrm{WF}_a(\Lambda^\pm)'$. By (12.8), we have for $\chi \in C_0^\infty(\mathbb{R}^n)$

$$|w_u^\pm(\chi\varphi_z^\lambda)| \leq C(\overline{\chi\varphi_z}^\lambda\cdot\Lambda^\pm\chi\varphi_z^\lambda)^{\frac{1}{2}}, \tag{12.9}$$

$$\overline{\chi\varphi_z}^\lambda\cdot\Lambda^\pm\chi\varphi_z^\lambda = \langle\Lambda^\pm|\overline{\chi}\varphi_{\overline{z}}^\lambda \otimes \chi\varphi_z^\lambda\rangle.$$

Note that $\varphi_{z_1}^\lambda \otimes \varphi_{z_2}^\lambda = \varphi_{(z_1,z_2)}^\lambda$, with the obvious notation. Since $(X_0, X_0) \notin \mathrm{WF}_a(\Lambda^\pm)'$ we can, by Definition 12.2.1, find χ equal to 1 near x_0, a neighborhood W of ξ_0 in $\mathbb{C}^n$, and $C, \epsilon > 0$ such that

$$\langle\Lambda^\pm|\overline{\chi}\varphi_{\overline{z}}^\lambda \otimes \chi\varphi_z^\lambda\rangle \leq C\mathrm{e}^{\frac{\lambda}{2}\left((\mathrm{Im}z)^2 + (\mathrm{Im}\overline{z})^2 - \epsilon\right)}.$$

By (12.9), this implies that $X_0 \notin \mathrm{WF}_a(w_u^\pm)$. Using (12.5) one obtains the same result for the C^∞ wavefront set. □

THEOREM 12.4.2. *Let P an analytic Klein-Gordon operator on (M, g) and ω a pure, analytic Hadamard state for P. Then ω satisfies the* Reeh-Schlieder property, *i.e. if $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is the* GNS *triple of ω and $O \subset M$ is an open set, the space* $\mathrm{Vect}\{W_\omega(u)\Omega_\omega : u \in C_0^\infty(O)\}$ *is dense in $\mathcal{H}_\omega$.*

Proof. We will apply Proposition 4.9.5 for $\mathcal{Y} = \dfrac{C_0^\infty(M)}{PC_0^\infty(M)}$ and $\mathcal{Y}_1 = \dfrac{C_0^\infty(O)}{PC_0^\infty(O)}$. Let $u \in \mathcal{Y}^{\rm cpl}$ such that $\overline{u}\cdot\Lambda^+ f = \overline{u}\cdot\Lambda^- f = 0$, $\forall f \in C_0^\infty(O)$, i.e. $\mathrm{supp}\, w_u^\pm \subset M \setminus O$. By (12.6), $N(\mathrm{supp}\, w_u^\pm) \subset \mathrm{WF}_a(w_u^\pm)$, hence $N(\mathrm{supp}\, w_u^\pm) \times N(\mathrm{supp}\, w_u^\pm) \subset \mathrm{WF}_a(\Lambda^\pm)'$. This contradicts the fact that ω is an analytic Hadamard state, since it is impossible that both (x, ξ) and $(x, -\xi)$ belong to $\mathcal{N}^+$ or to $\mathcal{N}^-$. Therefore, $\partial\,\mathrm{supp}\, w_u^\pm = \emptyset$, i.e. $w^\pm = 0$. This implies that u is orthogonal to $C_0^\infty(M)$ for $(\cdot|\cdot)_\omega$, hence $u = 0$. □

REMARK 12.4.3. *Note that much weaker conditions than the Hadamard property of ω are sufficient to ensure that the Reeh-Schlieder property holds: it suffices that if $(X, X) \in \mathrm{WF}_a(\Lambda^\pm)'$, then $(-X, -X) \notin \mathrm{WF}_a(\Lambda^\pm)'$, where $-X = (x, -\xi)$ if $X = (x, \xi)$.*

12.5. Existence of analytic Hadamard states

The question of the existence of analytic Hadamard states cannot be settled as easily as in the C^∞ case. In fact, the deformation argument of Fulling, Narcowich and Wald presented in Section 8.9 relies on cutoff functions, and hence does not apply in the analytic case.

Strohmaier, Verch and Wollenberg [**SVW**, Theorem 6.3] proved that if (M, g) is *stationary*, then the vacuum and thermal states associated to the group of Killing isometries are analytic Hadamard states.

The following theorem, which essentially settles the existence question, is proved in [**GW5**] using a general Wick rotation argument.

THEOREM 12.5.1. *Let (M, g) be an analytic, globally hyperbolic spacetime having an analytic Cauchy surface. Let P be an analytic Klein-Gordon operator on (M, g). Then there exists a pure analytic Hadamard state for P.*

12.6. Wick rotation on analytic spacetimes

Let (M, g) be an analytic, globally hyperbolic spacetime and assume that Σ admits an analytic, space-like Cauchy surface. Let P an analytic Klein-Gordon operator on M.

Clearly the diffeomorphism $\chi : U \to V$ in Proposition 5.4.7 given by Gaussian normal coordinates to Σ is analytic. We have $\chi^* g = -dt^2 + h(t, x)dx^2$, where $h(t, x)dx^2$ is a t-dependent Riemannian metric on Σ, analytic in (t, x) on U.

One can moreover ensure, after an analytic conformal transformation, that the Riemannian manifold $(\Sigma, h(0, x)dx^2)$ is complete, see [**GW5**, Subsection 3.1].

After conjugation by an analytic function of the form $\mathrm{e}^{\mathrm{i}F}$, see Subsection 11.6.3, the pullback of P to U can be reduced to a model Klein-Gordon operator

$$P = \partial_t^2 + r(t, x)\partial_t + a(t, x, \partial_x),$$

as in Section 11.2.

12.6.1. The Wick rotated operator. The function $t \mapsto r(t, \cdot)$ and the differential operator $t \mapsto a(t, x, \partial_x)$ extend holomorphically in t in a neighborhood W of $\{0\} \times \Sigma$ in $\mathbb{C} \times \Sigma$. Therefore, there exists a neighborhood V of $\{0\} \times \Sigma$ in $\mathbb{R} \times \Sigma$ on which the *Wick rotated operator*

$$K := -\partial_s^2 - \mathrm{i}r(\mathrm{i}s, x)\partial_s + a(\mathrm{i}s, x, \partial_x) \tag{12.10}$$

obtained from P by the substitution $t = \mathrm{i}s$ is well defined and analytic in (s, x) on V. Shrinking V we can assume that V is invariant under the reflection $(s, x) \mapsto (-s, x)$. We have $\sigma_{\mathrm{pr}}(K) = \sigma^2 + \xi \cdot h(\mathrm{i}s, x)\xi$, hence after further shrinking V, we can also assume that K is *elliptic* on V.

Note that for the moment K has no realization as an unbounded operator. To fix such a realization, one introduces *Dirichlet boundary conditions* on the boundary of some open set $\Omega \subset V$. The natural way to do this is by sesquilinear form arguments. Namely, we set $\hat{h}(s, x) = (h(\mathrm{i}s, x)^* h(\mathrm{i}s, x))^{\frac{1}{2}}$, which is positive definite, and denote by $L^2(\Omega)$ the space $L^2(\Omega, |\hat{h}(s, x)|^{\frac{1}{2}} dxds)$. Similarly, we denote by $L^2(\Sigma; \mathbb{C}^2)$ the space $L^2(\Sigma, |h(0, x)|^{\frac{1}{2}} dx; \mathbb{C}^2)$.

Let $H_0^1(\Omega)$ be the closure of $C_0^\infty(\Omega)$ with respect to the norm

$$\|u\|^2_{H^1(\Omega)} = \int_\Omega \big(|\partial_s u|^2 + \partial_j \overline{u} h_0^{jk} \partial_k u + |u|^2\big)|h(0, x)|^{\frac{1}{2}} dxds,$$

and let

$$Q_\Omega(v, u) = (v|Ku)_{L^2(\Omega)}, \ \mathrm{Dom}\, Q_\Omega = C_0^\infty(\Omega).$$

One can show, see [**GW5**, Proposition 3.2], that one can choose Ω close enough to $\{0\} \times \Sigma$ so that Q_Ω is closeable on $C_0^\infty(\Omega)$ and its closure $\overline{Q}_\Omega$ is *sectorial* with domain $H_0^1(\Omega)$, see [**Ka**, Chapter 6] for terminology.

One denotes by K_Ω the closed operator associated to $\overline{Q}_\Omega$. One can show that $0 \notin \sigma(K_\Omega)$ if Ω is close enough to $\{0\}\times\Sigma$. This is deduced from the one-dimensional Poincaré inequality $\int_{-a}^{a} |\partial_s u|^2 ds \geq (\frac{\pi}{2a})^2 \int_{-a}^{a} |u|^2 ds$.

12.7. The Calderón projectors

The *Calderón projectors* are a well-known tool in the theory of elliptic boundary value problems. Let us first explain this in an informal way.

Let X a smooth manifold and $\Omega \subset X$ an open set with smooth boundary. If $\mathcal{F}(X) \subset \mathcal{D}'(X)$ is a space of distributions, we denote by $\overline{\mathcal{F}}(\Omega) \subset \mathcal{D}'(\Omega)$ the space of *restrictions* to Ω of elements in $\mathcal{F}(X)$. So, for example, $\overline{\mathcal{D}'}(\Omega)$ is the space of *extendable distributions* on Ω and any $u \in \overline{\mathcal{D}'}(\Omega)$ has an extension eu with $eu = 0$ in $X \setminus \Omega^{\rm cl}$.

Now let K be an elliptic, second-order differential operator on X. Let us assume that K has some realization as an unbounded operator, still denoted by K with $0 \notin \sigma(K)$. Set $\Omega^+ = \Omega$ and $\Omega^- = X \setminus \Omega^{\rm cl}$. If $u \in \overline{\mathcal{D}'}(\Omega^\pm)$ satisfies $Ku = 0$ in $\Omega^\pm$, then its trace

$$\gamma^\pm u = \begin{pmatrix} u\restriction_{\partial\Omega} \\ \partial_\nu u\restriction_{\partial\Omega} \end{pmatrix} \in \mathcal{D}'(\partial\Omega; \mathbb{C}^2)$$

is well defined, where ∂_ν is some fixed transverse vector field to $\partial\Omega$. Let

$$Z^\pm = \{f \in \mathcal{D}'(\partial\Omega; \mathbb{C}^2) : f = \gamma^\pm u, \text{for some } u \in \overline{\mathcal{D}'}(\Omega^\pm),\ Ku = 0\}.$$

Then Z^+, Z^- are complementary subspaces in $\mathcal{D}'(\partial\Omega)$. The *Calderón projectors* $C_\Omega^\pm$ are the projectors on $Z^\pm$ along $Z^\mp$.

Let us assume for example that $X = \mathbb{R}_s \times S$, where (S, h) is a compact Riemannian manifold, $K = -\partial_s^2 - \Delta_h + m^2$ and $\Omega^\pm = \mathbb{R}^\pm \times S$. Then if $u \in \overline{\mathcal{D}'}(\Omega^\pm)$ satisfies $Ku = 0$ in $\Omega^\pm$ we have $u(s, \cdot) = \mathrm{e}^{\mp s\epsilon} v(\cdot)$ for $v \in \mathcal{D}'(S)$ and $\epsilon^2 = -\Delta_h + m^2$. Further, we have $\gamma^\pm u = \begin{pmatrix} v \\ \pm\epsilon v \end{pmatrix}$ and an easy computation shows that

$$C_\Omega^\pm = \frac{1}{2} \begin{pmatrix} \mathbb{1} & \pm\epsilon^{-1} \\ \pm\epsilon & \mathbb{1} \end{pmatrix},$$

which are exactly the projections $c^\pm$ in (4.46) associated to the *vacuum state* for the ultra-static spacetime $(\mathbb{R}_t \times S, g)$, $g = -dt^2 + h(x)dx^2$ and the Klein-Gordon operator $-\Box_g + m^2$.

We now define the Calderón projectors in our concrete situation. We take $\Omega^\pm = \Omega \cap \{\pm s > 0\}$, set

$$\gamma u = \begin{pmatrix} u\restriction_\Sigma \\ -\partial_s u\restriction_\Sigma \end{pmatrix}, \quad u \in C^\infty(\Omega),$$

and denote by $\gamma^\pm$ the analogous trace operators defined on $\overline{C^\infty}(\Omega^\pm)$. Let also

$$\gamma^* f = \delta(s) \otimes f_0 + \delta'(s) \otimes f_1, \quad f = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} \in C_0^\infty(\Sigma)^2,$$

which is the formal adjoint of $\gamma : L^2(\Omega) \to L^2(\Sigma; \mathbb{C}^2)$, and

$$S = \begin{pmatrix} 2\mathrm{i}\partial_t d(0, y) & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix},$$

where $d(t, y) = |h(t, x)|^{1/4} |h(0, x)|^{-1/4}$.

DEFINITION 12.7.1. *The* Calderón projectors *for* K_Ω *are the operators*

$$C_\Omega^\pm := \mp\gamma^\pm K_\Omega^{-1}\gamma^* S.$$

Note that it is not a priori clear that $C_\Omega^\pm$ are well defined, even as maps from $C_0^\infty(\Sigma)^2$ to $\mathcal{D}'(\Sigma)^2$. Despite their name, it is even less clear whether $C_\Omega^\pm$ are projectors on suitable spaces. The first issue is fixed by the following result from [**GW5**], which is well known if $\Sigma = \partial\Omega^\pm$ is compact.

PROPOSITION 12.7.2. *The maps* $C_\Omega^\pm$ *belong to* $\Psi^\infty(\Sigma; M_2(\mathbb{C}))$. *In particular, they are well defined from* $C_0^\infty(\Sigma;\mathbb{C}^2)$ *to* $C^\infty(\Sigma;\mathbb{C}^2)$.

12.8. The Hadamard state associated to Calderón projectors

We recall that $q = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$.

THEOREM 12.8.1. *Let* $\lambda^\pm_{\mathrm{Wick}} = \pm q \circ C_\Omega^\pm$. *Then* $\lambda^\pm_{\mathrm{Wick}}$ *are the Cauchy surface covariances on* Σ *of a pure analytic Hadamard state* ω_{Wick} *for* P.

The proof that $\lambda^\pm_{\mathrm{Wick}}$ are the covariances of a quasi-free state is rather technical. It relies on various integration by parts formulas and also on the fact that $K_\Omega + K_\Omega^* \geq 0$. This positivity is a version of *reflection positivity* in this context.

The proof of the purity of ω_{Wick} is also quite delicate, since to show that $C_\Omega^\pm$ are projections, one has to give a meaning to $C_\Omega^\pm \circ C_\Omega^\pm$, which seems difficult in this very general situation. One has to use the characterization of quasi-free states in Proposition 4.9.4 and an approximation argument, see [**GW5**, Section 4].

The essential ingredient for establishing the analytic Hadamard property of ω_{Wick} is the following proposition, whose proof is sketched below.

PROPOSITION 12.8.2.

$$\mathrm{WF}_a(U_\Sigma C_\Omega^\pm f) \subset \mathcal{N}^\pm, \quad \forall f \in \mathcal{E}'(\Sigma)^2.$$

Proof. We prove the result for the + case. Let us set

$$v := -K_\Omega^{-1}\gamma^* S f, \quad g := \gamma^+ v = C_\Omega^+ f, \quad u := U_\Sigma C_\Omega^+ f,$$

where U_Σ is the Cauchy evolution operator for P. Let us assume for simplicity that P is defined and analytic in $I \times \Sigma$ for $I \ni 0$ an open interval, and that it extends holomorphically in t to $(I \times \mathrm{i}I) \times \Sigma$. This can easily be ensured by a localization argument. Writing $z = t + \mathrm{i}s$, we denote the holomorphic extension of P by P_z, and hence P by P_t and K by $P_{\mathrm{i}s}$. We set also

$$I^{\mathrm{r/l}} = I \cap \{\pm t > 0\}, \quad I^\pm = I \cap \{\pm s > 0\},$$
$$D = I \times \mathrm{i}I, \quad D^+ = I \times \mathrm{i}I^+, \quad D^{\mathrm{r/l}} = I^{\mathrm{r/l}} \times \mathrm{i}I.$$

Step 1:

we can write v as:

$$v(s,y) = v^{\mathrm{r}}(\mathrm{i}s + 0, y) - v^{\mathrm{l}}(\mathrm{i}s - 0, y),$$

with $v^{\mathrm{r/l}} \in \mathscr{O}_{\mathrm{temp}}(D^{\mathrm{r/l}}; \mathcal{D}'(\Sigma))$. We have

$$P_{\mathrm{i}s} v = \delta(s) \otimes h_0(x) + \delta'(s) \otimes h_1(x) \quad \text{on } I \times \Sigma.$$

Using that $\delta(s) = \dfrac{1}{2\mathrm{i}\pi}\Big(\dfrac{1}{s + \mathrm{i}0} - \dfrac{1}{s - \mathrm{i}0}\Big)$, this implies that $P_z v^{\mathrm{r/l}} = w$ in $D^{\mathrm{r/l}} \times \Sigma$, where

$$w(z,y) = \frac{1}{2\pi z} \otimes h_0(x) + \frac{1}{2\mathrm{i}\pi z^2} \otimes h_1(x) + r(z,x),$$

and $r(z,x) \in \mathscr{O}(D;\mathcal{D}'(\Sigma))$. Note that $w \in \mathscr{O}_{\text{temp}}(D^+;\mathcal{D}'(\Sigma))$. We now define distributions $u^{\text{r/l}}(t,x)$ on $I^{\text{r/l}} \times \Sigma$ by

$$u^{\text{r/l}}(t,x) := v^{\text{r/l}}(t+\text{i}0,y),$$

so that $P_t u^{\text{r/l}}(t,x) = P_z v^{\text{r/l}}(t+\text{i}0,x) = w(t+\text{i}0,x)$. In Fig. 5 below we explain the relation between v, $v^{\text{r/l}}$ and $u^{\text{r/l}}$, the arrows corresponding to boundary values.

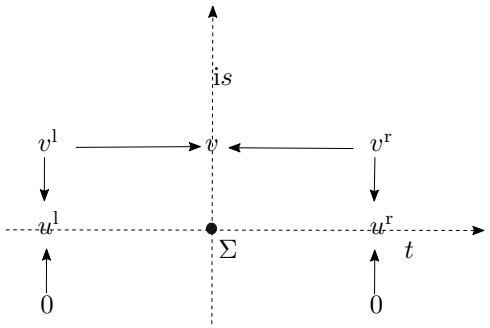


Fig. 5.

Since P_t is hyperbolic with respect to dt, we can extend $u^{\text{r/l}}$ as $\tilde{u}^{\text{r/l}} \in \mathcal{D}'(I \times \Sigma)$ with

$$P_t \tilde{u}^{\text{r/l}}(t,x) = w(t+\text{i}0,x), \quad \tilde{u}^{\text{r/l}}(t,x) = u^{\text{r/l}}(t,x) \text{ in } I^{\text{r/l}}.$$

By Proposition 12.2.4, $\text{WF}_a(w(t+\text{i}0,x)) \subset \{\tau \geq 0\}$ and $\text{WF}_a u^{\text{r/l}} \subset \{\tau \geq 0\}$ over $I^{\text{r/l}} \times \Sigma$, and so by Theorem 12.2.3 we know that $\text{WF}_a \tilde{u}^{\text{r/l}} \subset \{\tau \geq 0\}$ over $I \times \Sigma$.

One can then deduce from Martineau's edge of the wedge theorem that there exist $\tilde{v}^{\text{r/l}}(z,x) \in \mathscr{O}_{\text{temp}}(D^+;\mathcal{D}'(\Sigma))$ such that $\tilde{u}^{\text{r/l}}(t,x) = \tilde{v}^{\text{r/l}}(t+\text{i}0,x)$, $P_z \tilde{v}^{\text{r/l}} = w$ and $\tilde{v}^{\text{r/l}}(z,x) = v^{\text{r/l}}(z,x)$ for $z \in D^+ \cap D^{\text{r/l}}$.

Now let $\tilde{v}(z,x) = \tilde{v}^{\text{r}}(z,x) - \tilde{v}^{\text{l}}(z,x) \in \mathscr{O}_{\text{temp}}(D^+;\mathcal{D}'(\Sigma))$ and $\tilde{u} = \tilde{v}(t+\text{i}0,x)$. We have $P_z \tilde{v} = 0$ hence $P_t \tilde{u} = 0$ and $\text{WF}_a(\tilde{u}) \subset \{\tau \geq 0\}$, and so $\text{WF}_a(\tilde{u}) \subset \mathcal{N}^+$ by microlocal ellipticity.

It remains to check that $\tilde{u} = U_\Sigma C^+_\omega f$ or, equivalently, that $\varrho_\Sigma u = \gamma^+ v$, which will complete the proof of the proposition.

Note that since $\tilde{v}(z,x) = \tilde{v}^{\text{r}}(z,x) - \tilde{v}^{\text{l}}(z,x)$, we have $v(s,x) = \tilde{v}(\text{i}s,x)$ for $s > 0$. If we were allowed to take directly the limit $s \to 0^+$, this would imply that $\tilde{u}(0,x) = \lim_{s\to 0^+} \tilde{v}(\text{i}s,x) = \lim_{s\to 0^+} v(0,x)$, and similarly $\text{i}^{-1}\partial_t \tilde{u}(0,x) = \lim_{s\to 0^+} p_s v(0,x)$ i.e. $\varrho_\Sigma \tilde{u} = \gamma^+ v = C^+_\Omega f$.

To justify this computation we use the fact that $\tilde{u} \in C^\infty(I;\mathcal{D}'(\Sigma))$, which in turn follows from the fact that $P_t \tilde{u} = 0$. If $\varphi \in C^\infty_0(\Sigma)$, then we have $\langle \tilde{u}(t,\cdot)|\varphi\rangle = \lim_{\epsilon\to 0^+} \langle \tilde{v}(t+\text{i}\epsilon,\cdot)|\varphi\rangle$ in $\mathcal{D}'(I)$. Since $\langle \tilde{u}(t,\cdot)|\varphi\rangle \in C^\infty(I)$, we actually have $\langle \tilde{u}(t,\cdot)|\varphi\rangle = \lim_{\epsilon\to 0^+} \langle \tilde{v}(t+\text{i}\epsilon,\cdot)|\varphi\rangle$ in $C^\infty(I)$, which justifies the above computation. □

12.9. Examples

We conclude this chapter by giving some explicit examples of Calderón projectors and of the quasi-free state they generate in the ultra-static case. We have then

$$P = \partial_t^2 + \epsilon^2, \quad K = -\partial_s^2 + \epsilon^2, \text{ for } \epsilon = (-\Delta_h + m^2)^{\frac{1}{2}}.$$

One can realize K as a selfadjoint operators in various ways. Let us list a few examples.

12.9.1. Boundary conditions at infinity. Let K_∞ the natural selfadjoint realization of K on $L^2(\mathbb{R})\otimes L^2(\Sigma)$. We saw in Section 12.7 that the associated Calderón projectors for $\Omega^+=\mathbb{R}^+\times\Sigma$ are

$$C^\pm_\infty=\frac{1}{2}\begin{pmatrix}\mathbb{1} & \pm\epsilon^{-1}\\ \pm\epsilon & \mathbb{1}\end{pmatrix},$$

and the associated state is the vacuum $\omega_{\rm vac}$ for P.

12.9.2. Dirichlet boundary conditions. Let now K_T be the selfadjoint realization of K on $L^2(\,]-T,T\,[\,)\otimes L^2(\Sigma)$ with Dirichlet boundary conditions on $s=\pm T$. We can easily compute K_T^{-1}, namely $K_T^{-1}v=u-r$, where

$$u(s)=(2\epsilon)^{-1}\int_{-\infty}^{+\infty}\Big(\theta(s-s')\mathrm{e}^{-(s-s')\epsilon}+\theta(s'-s)\mathrm{e}^{(s-s')\epsilon}\Big)v(s')ds',$$

and

$$r(s)=(2\epsilon)^{-1}\Big(\mathrm{e}^{4T\epsilon}-1\Big)^{-1}\Big(\mathrm{e}^{(2T-s)\epsilon}v^+-\mathrm{e}^{s\epsilon}v^+-\mathrm{e}^{-s\epsilon}v^-+\mathrm{e}^{(s+2T)\epsilon}v^-\Big),$$

$$v^\pm=\int_{-T}^{T}\mathrm{e}^{\pm s'\epsilon}v(s')ds'.$$

Taking $\Omega^+=\,]0,T\,[\,\times\Sigma$, the Calderón projectors are

$$C^\pm_T=\frac{1}{2}\begin{pmatrix}\mathbb{1} & \pm\epsilon^{-1}\mathrm{th}(T\epsilon)\\ \pm\epsilon\coth(T\epsilon) & \mathbb{1}\end{pmatrix}. \tag{12.11}$$

The associated state is a pure Hadamard state for P. If $m=0$ the infrared singularity at $\epsilon=0$ is smoothed out by the Dirichlet boundary condition. When $T\to\infty$, $C^\pm_T$ converge to $C^\pm_\infty$.

12.9.3. β-periodic boundary conditions. Let $\mathbb{S}_\beta=\,]-\beta/2,\beta/2\,[$ with endpoints identified be the circle of length β and $K^{\rm per}_\beta$ be the β-periodic realization of K on $L^2(\mathbb{S}_\beta)\otimes L^2(\Sigma)$. The kernel of $(K^{\rm per}_\beta)^{-1}$ has the following well-known expression:

$$(K^{\rm per}_\beta)^{-1}(s)=\frac{\mathrm{e}^{-s\epsilon}+\mathrm{e}^{(s-\beta)\epsilon}}{2\epsilon(1-\mathrm{e}^{-\beta\epsilon})},\quad s\in\,]\,0,\beta\,[,$$

extended to $s\in\mathbb{R}$ by β-periodicity. Let us take $\Omega^+=\,]\,0,\beta/2\,[$. Since $\partial\Omega^+=\{0\}\times\Sigma\cup\{\beta/2\}\times\Sigma$, we can identify $C^\infty_0(\partial\Omega^+;\mathbb{C}^2)$ with $C^\infty_0(\Sigma;\mathbb{C}^2)\oplus C^\infty_0(\Sigma;\mathbb{C}^2)$ by writing $f\in C^\infty_0(\partial\Omega^+;\mathbb{C}^2)$ as $f=f^{(0)}\oplus f^{(\beta/2)}$ for $f^{(i)}\in C^\infty_0(\Sigma;\mathbb{C}^2)$. We set

$$T(f^{(0)}\oplus f^{(\beta/2)})=f^{(\beta/2)}\oplus f^{(0)}$$

and denote by $\epsilon_{\rm d}$ the operator $\epsilon\oplus\epsilon$.

Then an easy computation shows that the Calderón projectors are:

$$C^\pm_\beta=\frac{1}{2}\begin{pmatrix}\mathbb{1} & \pm\epsilon_{\rm d}^{-1}(\coth(\frac{\beta}{2}\epsilon_{\rm d}))+T\mathrm{sh}^{-1}((\frac{\beta}{2}\epsilon_{\rm d}))\\ \pm\epsilon_{\rm d}(\coth(\frac{\beta}{2}\epsilon_{\rm d}))-T\mathrm{sh}^{-1}((\frac{\beta}{2}\epsilon_{\rm d})) & \mathbb{1}\end{pmatrix}.$$

Since $\partial\Omega^+$ consists of two copies of Σ, the projections $C^\pm_\beta$ are associated to a pure quasi-free state on the doubled phase space $(\mathcal{Y}_{\rm d},q_{\rm d})$ obtained from $(\mathcal{Y},q)=(C^\infty_0(\Sigma;\mathbb{C}^2),q)$, see Subsection 4.8.4.

If we restrict this state to $\mathrm{CCR}(\mathcal{Y},q)$, we obtain the *thermal state* ω_β at temperature β^{-1} for P, see Subsection 4.10.3.

CHAPTER 13

Hadamard states and characteristic Cauchy problem

In this chapter we describe a different construction of Hadamard states which relies on the use of *characteristic cones* and is due to Moretti [**Mo1, Mo2**]. The original motivation was to construct a canonical Hadamard state on spacetimes with some asymptotic symmetries. The class of spacetimes considered are those that are *asymptotically flat* at past (or future) *null infinity*. After a conformal transformation, the original spacetime (M, g) can be regarded as the interior of a future light cone $\mathscr{I}^-$, called the *past null infinity* in some larger space time $(\tilde{M}, \tilde{g})$, where $\tilde{g} = \Omega^2 g$ in M.

Since $\mathscr{I}^-$ is a null hypersurface, any normal vector field to $\mathscr{I}^-$ is also tangent to $\mathscr{I}^-$, so the trace on $\mathscr{I}^-$ of a solution $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$ of the Klein-Gordon equation in M consists of a single scalar function. The symplectic form on $\mathrm{Sol}_{\mathrm{sc}}(P)$ induces a *boundary symplectic form* $q_{\mathscr{I}^-}$ on a space $\mathcal{H}_{\mathscr{I}^-}$ of scalar functions on $\mathscr{I}^-$. One can use this boundary symplectic space as a new phase space and a quasi-free state $\omega_{\mathscr{I}^-}$ on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{H}_{\mathscr{I}^-}, q_{\mathscr{I}^-})$ induces a quasi-free state ω on $\mathrm{CCR}(P)$.

The Hadamard condition for ω is rather easy to characterize in terms of $\omega_{\mathscr{I}^-}$, since the covariances of $\omega_{\mathscr{I}^-}$ are simply scalar distributions, and not 2×2 matrices as in the case of a space-like Cauchy surface Σ considered in Chapter 11.

The past null infinity in an asymptotically flat spacetime (M, g) is traditionally denoted by $\mathscr{I}^-$ and the metric $\tilde{g}$ and conformal factor Ω induce on $\mathscr{I}^-$ a *conformal frame*, consisting of a degenerate Riemannian metric $\tilde{h}$ on $\mathscr{I}^-$ and a vector field n. The group of diffeomorphisms of $\mathscr{I}^-$ leaving the set of conformal frames invariant is called the (*Bondi-Metzner-Sachs*) BMS *group*, which is interpreted as the group of asymptotic symmetries of M at past null infinity.

At the end of this chapter we give a short description of these objects. The BMS group G_{BMS} acts on $\mathcal{H}_{\mathscr{I}^-}$ by symplectic transformations, and a natural state on $\mathscr{I}^-$ should be invariant under the action of G_{BMS}. We will describe the construction of this state due to Moretti [**Mo1**].

13.1. Klein-Gordon fields inside future lightcones

13.1.1. Future lightcones. Let (M, g) a globally hyperbolic spacetime and $p \in M$ a base point. It is known, see [**W1**, Section 8.1], that on any spacetime M, $I_+(p)$ is open with $I_+(p)^{\mathrm{cl}} = J_+(p)^{\mathrm{cl}}$, $\partial I_+(p) = \partial J_+(p)$. Moreover, any causal curve from p to $q \in \partial I_+(p)$ must be a null geodesic. Since (M, g) is globally hyperbolic, $J_+(p)$ is closed, see [**BGP**, Appendix A.5], hence $I_+(p)^{\mathrm{cl}} = J_+(p)$.

We set

$$M_0 := I_+(p), \quad C := \partial I_+(p) \setminus \{p\}, \tag{13.1}$$

so C is the *future lightcone* from p, with its tip p removed and M_0 is the interior of C. The following results on the causal structure of M_0 are due to Moretti [**Mo1**, Theorem 4.1] and [**Mo2**, Lemma 4.3].

PROPOSITION 13.1.1. *The spacetime (M, g_0) is globally hyperbolic. Moreover*

$$J_+^{M_0}(K) = J_+^M(K), \quad J_-^{M_0}(K) = J_-^M(K) \cap M_0, \ \ \forall K \subset M_0. \tag{13.2}$$

PROPOSITION 13.1.2. *Let $K \Subset M_0$. Then there exists a neighborhood U of p in M such that no null geodesic starting from K intersects $C^{\rm cl} \cup U$.*

13.1.2. Klein-Gordon fields in M_0. Let $P = P(x, \partial_x)$ be a Klein-Gordon operator in M, $G_{\rm ret/adv}$ its retarded/advanced inverses and $P_0 = P_0(x, \partial_x)$ the restriction of P to M_0. From Proposition 13.1.1 we obtain immediately that the retarded/advanced inverses $G_{\rm ret/adv,0}$ of P_0 are the restrictions of $G_{\rm ret/adv}$ to M_0 and hence

$$G_0 = G\restriction_{M_0 \times M_0},$$

where G, G_0 are the Pauli-Jordan functions for P, P_0.

13.1.3. Null coordinates near C. Clearly, the cone C will in general not be an embedded submanifold of M, due to the possible presence of caustics.

Let us introduce some assumptions from **[GW2]**, which avoid this problem and are a version of the notion of *asymptotic flatness* (with past time infinity). We will come back to this notion in Section 13.5.

We assume that there exists a function $f \in C^\infty(M)$ such that

(13.3)

(1) $C \subset f^{-1}(\{0\}), \quad \nabla_a f \neq 0$ on $C, \quad \nabla_a f(p) = 0, \quad \nabla_a \nabla_b f(p) = -2 g_{ab}(p),$

(2) the vector field $\nabla^a f$ is complete on C.

It follows that C is a smooth hypersurface, although $C^{\rm cl}$ is not. Moreover, since C is a null hypersurface, $\nabla^a f$ is tangent to C.

To construct null coordinates near C, one needs to fix a compact submanifold $S \subset C$, of codimension 2 in M, such that $\nabla^a f$ is transverse to S. Then S is diffeomorphic to $\mathbb{S}^{n-2}$ and C to $\mathbb{R} \times \mathbb{S}^{n-2}$.

One can then, see e.g., **[GW2**, Lemmas 2.5, 2.6**]**, prove the following standard fact:

PROPOSITION 13.1.3. *There exist a neighborhood U of C in M and a diffeomorphism*

$$\begin{aligned} \chi : \ \ & U \longrightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{S}^{n-2} \\ & x \longmapsto (f(x), s(x), \theta(x)) \end{aligned}$$

such that

$$(\chi^{-1})^*(\nabla^a f \restriction_C) = -\partial_s, \quad \big((\chi^{-1})^* g\big)\restriction_C = -2 df ds + h_{ij}(s,\theta) d\theta^i d\theta^j, \tag{13.4}$$

where $h_{ij}(s,\theta) d\theta^i d\theta^j$ is a smooth s-dependent Riemannian metric on $\mathbb{S}^{n-2}$. Moreover, if $h_{ij}(\theta) d\theta^i d\theta^j$ is the standard metric on $\mathbb{S}^{n-2}$ one has

$$|h_{ij}(s,\theta)|^{\frac{1}{2}} = O(\mathrm{e}^{2s(n-2)}) |h_{ij}(\theta)|^{\frac{1}{2}} \ \ \text{for } s \in]-\infty, R], \ R > 0. \tag{13.5}$$

The above diffeomorphism depends only on f satisfying (13.3) and on the choice of the submanifold S.

Restricting χ to C gives a diffeomorphism $\chi\restriction_C \colon C \to \mathbb{R} \times \mathbb{S}^{n-2}$ that is rather easy to describe: let us first fix normal coordinates $(y^0, \overline{y})$ at p such that in a neighborhood of p, $C = \{(y^0)^2 - |\overline{y}|^2 = 0, \ y^0 > 0\}$.

If $\{\phi_t\}_{t \in \mathbb{R}}$ is the flow of $\nabla^a f$ on C, we define $s = s(x)$ for $x \in C$ by $x = \phi_s(x')$ for a unique $x' \in S$. One sees that $\phi_t(x') \to p$ when $t \to -\infty$ and one defines $\theta(x) = \lim_{t \to -\infty} \frac{\overline{y}}{|\overline{y}|}(\phi_t(x')) \in \mathbb{S}^{n-2}$.

13.1.4. Change of gauge. One can view the choice of (f, S) as the choice of a *gauge*. If $\omega \in C^\infty(M)$ is such that $\omega > 0$ on C and $\omega(p) = 1$, then $f' = \omega f$ also satisfies (13.3). Let also S' be another submanifold transverse to $\nabla^a f$.

If $\chi' : U' \to \mathbb{R} \times \mathbb{R} \times \mathbb{S}^{n-2}$ is the corresponding diffeomorphism in Proposition 13.1.3 one can easily see that

$$\psi := (\chi' \restriction_C) \circ (\chi \restriction_C)^{-1} : (s, \theta) \longmapsto (s'(s, \theta), \theta),$$

for some function $s'(s, \theta)$ on $\mathbb{R} \times \mathbb{S}^{n-2}$. Explicitly, if S' is given in the (s, θ) coordinates by $\{s = b(\theta)\}$, one has

$$s'(s, \theta) = -b(\theta) + \int_0^s \omega^{-1}(\sigma, \theta) d\theta. \tag{13.6}$$

The map ψ is quite similar to the so-called *supertranslations*, see Section 13.5. If $h'(s', \theta')d\theta'^2$ is the corresponding metric in (13.4), then $h' d\theta'^2 = (\psi)^* h d\theta^2$.

13.2. The boundary symplectic space

Let us consider the symplectic space $(\mathrm{Sol}_{\mathrm{sc}}(P_0), q)$. Clearly, any solution $\phi_0 \in \mathrm{Sol}_{\mathrm{sc}}(P_0)$ extends to a solution $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$, hence its trace on C

$$\varrho_C \phi_0 := \phi_0 \restriction_C, \tag{13.7}$$

is well defined. Note that since C is null, a vector field n normal to C is also tangent to C, so $\partial_n \phi_0 \restriction_C$ is determined by $\phi_0 \restriction_C$.

We would like to introduce a *boundary symplectic space* $(\mathcal{H}_C, q_C)$ of functions on C which will play the role of $(C_0^\infty(\Sigma; \mathbb{C}^2), q)$ for a Cauchy surface Σ in M_0 and such that

$$\varrho_C : (\mathrm{Sol}_{\mathrm{sc}}(P_0), q) \longrightarrow (\mathcal{H}_C, q_C)$$

is *weakly symplectic*, i.e. such that $\varrho_C^* q_C \varrho_C = q$. Note that this implies that ϱ_C is injective. The map ϱ_C is sometimes called a *bulk-to-boundary correspondence*.

The space $\mathcal{H}_C$ should be small enough to admit interesting quasi-free states, and depend only on C, not on a particular gauge (f, S).

Let us denote by $H^\infty_{f,S}$ the set of $g \in \mathcal{D}'(C)$ such that

$$\int_{\mathbb{R} \times \mathbb{S}^{n-2}} \left| \partial_s^\alpha \partial_\theta^\beta g(s, \theta) \right|^2 \left| h(s, \theta) \right|^{\frac{1}{2}} ds d\theta < \infty, \ \ \forall (\alpha, \beta) \in \mathbb{N}^{n-1}.$$

equipped with its Fréchet space topology and

$$H^\infty_{f,S,R} := \{ g \in H^\infty_{f,S} : \operatorname{supp} g \subset]-\infty, R], \ R \in \mathbb{R} \}.$$

The space $H^\infty_{f,S}$ depends on (f, S), but the inductive limit

$$\mathcal{H}_C := \bigcup_{R \in \mathbb{R}} H^\infty_{f,S,R}$$

does not. This can be verified quite easily using (13.6) and the estimates in [**GW2**, Lemmas 2.7, 2.8].

Proposition 13.2.1. *Set*

$$\overline{g}_1 \cdot q_C g_2 := \mathrm{i} \int_{\mathbb{R} \times \mathbb{S}^{n-2}} \left(\partial_s \overline{g}_1 g_2 - \overline{g}_1 \partial_s g_2 \right) |h(s, \theta)|^{\frac{1}{2}} ds d\theta, \quad g_1, g_2 \in \mathcal{H}_C. \tag{13.8}$$

Then:

(1) *q_C is well defined and independent on the choice of the gauge (f, S),*
(2) *$(\mathcal{H}_C, q_C)$ is a Hermitian space,*
(3) *$\varrho_C : (\mathrm{Sol}_{\mathrm{sc}}(P_0), q) \to (\mathcal{H}_C, q_C)$ is unitary.*

Proof. q_C is clearly well defined on $\mathcal{H}_C$. Its independence on the choice of the gauge follows from the discussion of changes of gauge in Subsection 13.1.4.

Let us now prove (2). We denote by $m(\theta)d\theta^2$ the canonical metric on $\mathbb{S}^{n-2}$ and set

$$Ug(s,\theta) = |m|^{-1/4}|h|^{1/4} g \circ (\chi\restriction_C)^{-1}(s,\theta). \tag{13.9}$$

We have

$$\overline{g}_1 \cdot q_C g_2 = \mathrm{i}^{-1} \int_{\mathbb{R}\times\mathbb{S}^{n-2}} \big(\overline{\partial_s U g}_1 U g_2 - \overline{U g}_1 \partial_s U g_2\big)|m|^{\frac{1}{2}}(\theta) ds d\theta.$$

We can integrate by parts in s with no boundary terms since $Ug \to 0$ when $s \to -\infty$ and $\operatorname{supp} Ug \subset]-\infty, R]$ and obtain that

$$\overline{g}_1 \cdot q_C g_2 = 2\mathrm{i}^{-1} \int_{\mathbb{R}\times\mathbb{S}^{n-2}} \overline{U g}_1 \partial_s U g_2 |m|^{\frac{1}{2}}(\theta) ds d\theta. \tag{13.10}$$

Hence, if $\overline{g}_1 \cdot q_C g_2 = 0$ for all $g_1 \in \mathcal{H}_C$, we have $\partial_s U g_2 = 0$, and so $Ug_2 = 0$.

Now let us prove (3). We first show that ϱ_C maps $\mathrm{Sol}_{\mathrm{sc}}(P_0)$ into $\mathcal{H}_C$. Let us verify that

$$\varrho_C : C_0^\infty(M) \longrightarrow \mathcal{H}_C \quad \text{continuously.} \tag{13.11}$$

This can be easily deduced from [**GW2**, Lemma 2.8]. Next, if $\phi_0 \in \mathrm{Sol}_{\mathrm{sc}}(P_0)$ with $\operatorname{supp}\phi_0 \subset J^{M_0}(K)$ for some $K \Subset M_0$, then we can extend ϕ_0 as $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$ with $\operatorname{supp}\phi \subset J(K)$ and $\operatorname{supp}\phi \cap C \subset (J_+(K) \cap J_+(p)) \cup J_-(K) \cap J_+(p)$. The first set is empty by Proposition 13.1.1, the second is compact by Lemma 5.4.3. Therefore, $\varrho_C \phi_0 = \varrho_C u$ for some $u \in C_0^\infty(M)$ hence belongs to $\mathcal{H}_C$.

We now fix a Cauchy surface Σ in M_0 and pick $\phi_1, \phi_2 \in \mathrm{Sol}_{\mathrm{sc}}(P_0)$, $g_i = \varrho_C \phi_i$. For $J_a(\phi_1, \phi_2)$ as in Subsection 5.5.2 we have $\overline{\phi}_1 \cdot q\phi_2 = \int_\Sigma J_a(\phi_1,\phi_2) n^a dVol_h$. Applying the Gauss formula as in Subsection 5.2.4 using the coordinates (f, s, θ) on C, we obtain that $\overline{\phi}_1 \cdot q\phi_2 = \overline{g}_1 \cdot q_C g_2$.

To justify the application of the Gauss formula to the non-smooth surface C^{cl}, it suffices to replace C^{cl} in an ϵ-neighborhood of p by a piece of a smooth Cauchy surface in M, the contribution of the integral on this part tends then to 0 when $\epsilon \to 0$. □

13.3. The Hadamard condition on the boundary

Let ω_C a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{H}_C, q_C)$, with covariances $\lambda_C^\pm$. We will call ω_C a *boundary state*. From Proposition 13.2.1 we see that ω_C induces a state ω_0 for $\mathrm{CCR}(P_0)$, called the induced *bulk state*, by setting

$$\Lambda_0^\pm := (\varrho_C \circ G_0)\lambda_C^\pm(\varrho_C \circ G_0). \tag{13.12}$$

We would like to give sufficient conditions on $\lambda_C^\pm$ which ensure that the induced state ω_0 is a Hadamard state.

Recall that we use the density $dVol_g$ to identify distributions with distributional densities on M_0. Similarly, we use the density $|h(s,\theta)|^{\frac{1}{2}} ds d\theta$ to identify distributions with distributional densities on C. Changing the gauge (f, S) amounts to multiplying distributions on C by a smooth, non-zero function hence does not change their wavefront set.

We will denote by $X = (x, \xi)$ resp. $Y = (y, \eta)$ the elements of $T^*X \setminus o$ resp. $T^*C \setminus o$. If necessary, we introduce near C the local coordinates (f, s, θ) as in Proposition 13.1.3, which we will denote by $(r, s, \overline{y})$, the dual variables being $(\varrho, \sigma, \overline{\eta})$.

Let $i^* : T^*_C M \to T^*C$ be the pullback by the injection $i : C \to M$ and recall that $N^*C = (i^*)^{-1}(o)$ is the conormal bundle of C in M, see Subsection 7.2.4. Recall

also that $\mathcal{N}^{\pm} \subset T^*M \setminus o$ are the two connected components of the characteristic manifold $\mathcal{N}$ of p.

LEMMA 13.3.1. *Consider the function $F(y,\eta) = \eta\cdot\nabla^a f(y)$ on T^*C and denote*

$$T^*C^{\pm} := \{Y \in T^*C : \pm F(Y) > 0\}, \quad T^*C^0 := \{Y \in T^*C : F(Y) = 0\}. \tag{13.13}$$

Then

(1) *$i^* : T^*_C M \cap \mathcal{N}^{\pm} \longrightarrow T^*C^{\pm}$ is bijective.*
(2) *$(i^*)^{-1}(T^*C^0) \cap \mathcal{N} = N^*C$,*
(3) *For $Y \in T^*C$, $X \in T^*M$ let us write $Y \sim X$ if $Y \in T^*C^{\pm}$ and $(i^*)^{-1}(Y) \sim X$. Let $\chi, \psi \in C_0^\infty(M)$ with $p \notin \operatorname{supp}\psi$. Then $\mathrm{WF}(\varrho_C \psi G \chi)' \subset \{(Y,X) : Y \sim X, x \in M_0\}$.*

The sets $T^*C^{\pm}$, T^*C^0 are clearly independent on the choice of f.

Proof. Let us use the above coordinates, so that $F(Y) = \sigma$. By Proposition 13.1.3 we have

$$p(X) = -2\varrho\sigma + h(0,\overline{y},\overline{\eta}), \quad X \in T^*_C M. \tag{13.14}$$

for $h(s,\overline{y},\overline{\eta}) = \overline{\eta}\cdot h^{-1}(s,\overline{y})\overline{\eta}$ and $N^*C = \{r = \sigma = \overline{\eta} = 0\}$. The proof of (1) and (2) is then easy. Let us prove (3). Since $p \notin \operatorname{supp}\psi$, the singularity of C at p is harmless. We check that $\mathrm{WF}(\varrho_C)' = \{(Y,X) \in T^*C \setminus o \times T^*M \setminus o : Y = i^*X\}$ and know that $\mathrm{WF}(\psi G\chi)' \subset \{(X_1,X_2) : X_1 \sim X_2, x_2 \in M_0\}$, see Proposition 7.4.4. Then we apply the composition rule in Subsection 7.2.8. □

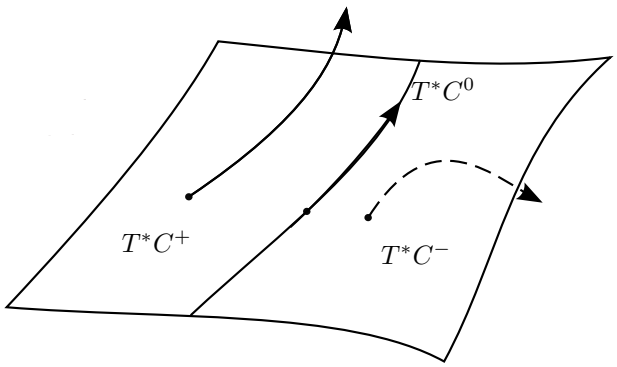


Fig. 6

THEOREM 13.3.2. *Let $\lambda_C^{\pm}$ be the covariances of a boundary state ω_C. Assume that $\lambda_C^{\pm} : \mathcal{H}_C \to \mathcal{H}_C^*$ are continuous and let*

$$\Lambda_0^{\pm} = (\varrho_C \circ G_0)^* \lambda_C^{\pm} (\varrho_C \circ G_0).$$

Then

(1) *$\Lambda_0^{\pm} \in \mathcal{D}'(M_0 \times M_0)$ are the spacetime covariances of a quasi-free state ω_0 for P_0.*
(2) *Assume that*

$$\mathrm{WF}(\lambda_C^{\pm})' \cap T^*C^{\mp} \times T^*C = \emptyset. \tag{13.15}$$

Then the bulk state ω_0 is a Hadamard state for P_0.

Proof. Assertion (1) follows from (13.11).

The proof of assertion (2) relies on a idea due to Moretti [**Mo2**], which allows to avoid the difficulties caused by the tip p of C. Note first that since $\lambda_C^{\pm} = \lambda_C^{\pm *}$ we deduce from (13.15) that

$$\mathrm{WF}(\lambda_C^{\pm})' \subset (T^*C^{\pm} \cup T^*C^0) \times (T^*C^{\pm} \cup T^*C^0). \tag{13.16}$$

It clearly suffices to estimate $\mathrm{WF}(\chi\Lambda_0^\pm\chi)'$ for $\chi \in C_0^\infty(M_0)$.

Observe first that $\varrho_C G_0\chi = \varrho_C G\chi$ since $G_0 = G\restriction_{M_0\times M_0}$. By the support property of G, we can pick $\psi \in C_0^\infty(M)$ such that $\varrho_C G\chi = \varrho_C\psi G\chi$. By Proposition 13.1.2, we can split ψ as $\psi_0 + \psi_\infty$, where $\psi_i \in C_0^\infty(M)$, $\psi_0 = 1$ near p, and no null geodesics from $\operatorname{supp}\chi$ intersect C in $\operatorname{supp}\psi_0$. Using that $\mathrm{WF}(G)' \subset \mathcal{C}$ we obtain that $\psi_0 G\chi : \mathcal{D}'(M_0) \to C_0^\infty(M)$ continuously, hence

$$\varrho\psi_0 G\chi : \mathcal{D}'(M) \longrightarrow \mathcal{H}_C$$

continuously, by (13.11). Since by assumption $\lambda_C^\pm : \mathcal{H}_C \to \mathcal{H}_C^*$ is continuous, in the definition of $\Lambda_0^\pm$ we can replace $\varrho_C G\chi$ by $\varrho_C\psi_\infty G\chi$, modulo a smoothing operator on M_0.

From Lemma 13.3.1 we know that

$$\mathrm{WF}(\varrho_C\psi_\infty G\chi)' \subset \{(Y,X) : Y \sim X, x \in M_0\},$$
$$\mathrm{WF}((\varrho_C\psi_\infty G\chi)^*)' \subset \{(X,Y) : Y \sim X, x \in M_0\}.$$

We observe that if $Y \sim X$ for $x \in M_0$, then $Y \notin T^*Y^0$. Indeed, if we assume that $Y \in T^*Y^0$ and $Y = i^*X'$ for $X' \sim X$, then necessarily $X' \in N^*C$, by Lemma 13.3.1. Since C is null, N^*C is invariant under the Hamiltonian flow of p, hence $X \in N^*C$ and $x \in C$, which is a contradiction.

This implies that we can find a pseudodifferential operator $Q \in \Psi_{\mathrm{c}}^0(C)$ with essential support (see Subsection 10.2.5) disjoint from T^*C^0 such that

$$\varrho_C\psi_\infty G\chi = Q\varrho_C\psi_\infty G\chi \quad \text{modulo a smoothing operator,}$$

and hence we can replace $\lambda_C^\pm$ by $Q^*\lambda_C^\pm Q$ with

$$\mathrm{WF}(Q^*\lambda_C^\pm Q) \subset T^*C^+ \times T^*C^+,$$

by (13.16). We can then apply twice the rules for composition of kernels in Subsection 7.2.8 and obtain by Lemma 13.3.1 that

$$\mathrm{WF}(\chi\Lambda_0^\pm\chi)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm,$$

i.e. condition (genHad) in Definition 8.4.1 is satisfied. By Thm 8.4.2 ω_0 is a Hadamard state for P_0. □

13.4. Construction of pure boundary Hadamard states

It is now rather easy to construct, for each given gauge (f, S), a boundary state ω_C which induces a Hadamard state ω_0 in M_0. We denote $L^2(\mathbb{R}\times\mathbb{S}^{n-2}; |m|^{\frac{1}{2}} d\theta ds)$ simply by $L^2(\mathbb{R}\times\mathbb{S}^{n-2})$ and recall that the map $U : \mathcal{H}_C \to L^2(\mathbb{R}\times\mathbb{S}^{n-2})$ was defined in (13.9).

Theorem 13.4.1. *Set*

$$\overline{g}_1 \cdot \lambda_C^\pm g_2 := 2(Ug_1 | \mathbb{1}_{\mathbb{R}^\pm}(D_s)|D_s|Ug_2)_{L^2(\mathbb{R}\times\mathbb{S}^{n-2})}.$$

Then the following holds:

(1) $\lambda_C^\pm$ *are the covariances of a pure quasi-free state* ω_C *on* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{H}_C, q_C)$.
(2) ω_C *depends on the choice of* f *but not of* S.
(3) ω_C *induces a Hadamard state* ω_0 *in* P_0.
(4) *Assume that* $\dim M \geq 4$. *Then the state* ω_0 *is* pure.

Proof. The fact that $\lambda_C^\pm$ are the covariances of a quasi-free state is obvious. To prove that ω_C is pure, we can apply Proposition 4.9.3. The completion of $U\mathcal{H}_C$ for the norm obtained from $\lambda_C^\pm$ is equal to $|D_s|^{\frac{1}{2}}L^2(\mathbb{R}\times\mathbb{S}^{n-2})$, on which $\mathbb{1}_{\mathbb{R}}^\pm(D_s)$ are complementary projections. This completes the proof of (1).

Changing the surface S amounts to replacing s by $s' = s - b(\theta)$ for some function b on $\mathbb{S}^{n-2}$, so $D_{s'} = D_s$, which proves (2). Statement (3) follows from Theorem

13.3.2 and the fact that in the coordinates (f,θ) on C, $T^*C^\pm$ is given by $\{\pm\sigma>0\}$. We refer the reader to **[GW2]** for details.

It remains to explain the proof of (4). The fact that ω_C is pure does not automatically ensure that ω_0 is pure. To prove this one has to show, again by Proposition 4.9.3, that $U\varrho_C\mathrm{Sol}_{\mathrm{sc}}(P_0)$ is dense in $|D_s|^{\frac{1}{2}}L^2(\mathbb{R}\times\mathbb{S}^{n-2})$.

This can be deduced from the solvability of the *characteristic Cauchy problem*

$$\left\{\begin{array}{l} P_0\phi=0 \text{ in } M_0,\\ \phi\restriction_C= g,\end{array}\right. \tag{13.17}$$

in energy spaces, by adapting a method due to Hörmander **[H6]**. We refer again the reader to **[GW2]**. The restriction to $n\geq 4$ comes from the use of a Hardy-type inequality on the cone C. □

13.5. Asymptotically flat spacetimes

The above method of constructing a bulk Hadamard state from a boundary state was originally developed by Moretti **[Mo1, Mo2]** for spacetimes that are *asymptotically flat* at past (or future) *null infinity*. In this case it is important to consider only the *conformal wave equation* and to assume that the spacetime dimension n is equal to 4 (the value of n is important when one takes the trace of some identities between tensors). In this subsection we would like to explain this notion and its relationship to the previous subsections. Our exposition below follows **[Mo2]**, **[DMP1]** or **[W1**, Section 11**]**, with some slight differences. For example, the conformal factor Ω already incorporates a change of gauge $\Omega\to\Omega'=\omega\Omega$ such that (13.18) is satisfied.

Definition 13.5.1. *A spacetime (M,g) is* asymptotically flat at past null infinity *if there exists another spacetime $(\tilde M,\tilde g)$ such that:*

(1) *$M\subset\tilde M$ is open, $\mathscr{I}^-:=\partial M$ is a smooth hypersurface homeomorphic to $\mathbb{R}\times\mathbb{S}^2$,*
(2) *there exists $\Omega\in C^\infty(\tilde M)$ with $\Omega>0$ on M, $\Omega=0, d\Omega\neq 0$ on $\mathscr{I}^-$,*
(3) *$\tilde g|_M=\Omega^2|_M g$ and $\mathscr{I}^-\cap J^{\tilde M}_+(M)=\emptyset$,*
(4) *$\tilde g^{ab}\widetilde\nabla_a\Omega\widetilde\nabla_b\Omega=0$ on $\mathscr{I}^-$,*
(5) *If $i:\mathscr{I}^-\to\tilde M$ is the canonical injection, then*

$$\begin{array}{l}\text{(i) } n^a=\widetilde\nabla^a\Omega \text{ is complete on } \mathscr{I}^-,\\ \text{(ii) } i^*(\widetilde\nabla_a\widetilde\nabla_b\Omega)=0.\end{array} \tag{13.18}$$

Let us denote by $\mathcal{M}$ the set of $(\tilde g,\Omega)$ such that conditions (2), (3), (4), (5) hold. From conditions (2), (3) we see that if $(\tilde g,\Omega)$ and $(\tilde g',\Omega')$ belong to $\mathcal{M}$, then there exists $\omega\in C^\infty(\tilde M)$, $\omega>0$ such that $\Omega'=\omega\Omega$, $\tilde g'=\omega^2\tilde g$. Moreover from conditions (4) and (5) it follows that $n^a\widetilde\nabla_a\omega=0$ on $\mathscr{I}^-$, see Lemma 13.5.3 below.

13.5.1. Conformal frames. Let $(\tilde g,\Omega)\in\mathcal{M}$. The manifold $\mathscr{I}^-$ is null for $\tilde g$ and is naturally equipped with the vector field n, which is tangent to $\mathscr{I}^-$ and with $\tilde h=\tilde g\restriction_{\mathscr{I}^-}$, which is a degenerate Riemannian metric with kernel spanned by n.

Definition 13.5.2. *The pair $(\tilde h,n)$ is called* the conformal frame *on $\mathscr{I}^-$ associated to $(\tilde g,\Omega)$. The set of all conformal frames associated to elements of $\mathcal{M}$ is denoted by $\mathcal{C}$.*

The above change of conformal factor $\Omega\to\Omega'=\omega\Omega$ is called a *gauge transformation* and induces the change $(\tilde h,n)\to(\tilde h',n')=(\omega^2\tilde h,\omega^{-1}n)$ on the associated conformal frames.

LEMMA 13.5.3. (1) *Let* $(\tilde{g},\Omega)\in\mathcal{M}$. *Then the associated conformal frame* $(\tilde{h},n)$ *satisfies:*

$$\mathrm{Ker}\,\tilde{h}(x)=\mathbb{R}n(x),\ x\in\mathscr{I}^-,\quad \mathcal{L}_n\tilde{h}=0,\ n \text{ is complete.} \tag{13.19}$$

(2) *Let* $(\tilde{h},n),(\tilde{h}',n')\in\mathcal{C}$. *Then there exists* $\omega\in C^\infty(\mathscr{I}^-)$ *with* $\omega>0$ *and* $\mathcal{L}_n\omega=0$ *such that* $(\tilde{h}',n')=(\omega^2\tilde{h},\omega^{-1}n)$.

Proof. Let us complete $x^0=\Omega$ with local coordinates x^i, $1\leq i\leq 3$, and remove the tildes to simplify notation. Then if $b=i^*(\nabla_i\nabla_j\Omega)$, we have $b_{ij}=-\Gamma^0_{ij}=-\frac{1}{2}g^{0k}(\partial_i g_{jk}+\partial_j g_{ik}-\partial_k g_{ij})$ since $g^{00}=0$ on $\mathscr{I}^-$. We compute the Lie derivative $\mathcal{L}_n h_{ij}=n^k\partial_k g_{ij}+\partial_i n^k g_{kj}+g_{ik}\partial_i n^k$. Using again that $g^{00}=0$, we see that $g^{0k}g_{kj}=\delta^0_j=0$. Taking derivatives of this identity we obtain that $b_{ij}=\frac{1}{2}\mathcal{L}_n h_{ij}$, which proves (1).

Let us prove (2). The existence of $\omega\in C^\infty(\mathscr{I}^-)$ with $\omega>0$ is obvious. To show that $\mathcal{L}_n\omega=0$ we compute

$$\mathcal{L}_n(\omega^2 h)=\omega^2\mathcal{L}_n h+2\omega\mathcal{L}_n(\omega)h,$$
$$\mathcal{L}_{\omega^{-1}n}(h)=\omega^{-1}\mathcal{L}_n h+d\omega^{-1}\otimes hn+hn\otimes d\omega^{-1},$$

whence

$$\mathcal{L}_{\omega^{-1}n}(\omega^2 h)=\omega\mathcal{L}_n h+2\mathcal{L}_n\omega h-d\ln\omega\otimes hn-hn\otimes d\ln\omega.$$

Using (1) for $(\tilde{h},n)$ and $(\tilde{h}',n')$ this implies that $\mathcal{L}_n\omega=0$. □

13.5.2. Bondi frames. Let now $(\tilde{h},n)$ be a conformal frame and $S,S'\subset\mathscr{I}^-$ be two smooth surfaces transverse to n. Since n is complete, its flow defines a diffeomorphism

$$\phi_{S'\leftarrow S}:S\longrightarrow S',$$

by identifying points in S and S' which are on the same integral curve of n. This diffeomorphism is independent on $(\tilde{h},n)$. Moreover, the flow of n defines a diffeomorphism

$$\begin{aligned}&\psi_{n,S}:\mathbb{R}_u\times S\longrightarrow\mathscr{I}^-,\ \text{with}\\ &S=\psi_{n,S}(\{0\}\times S),\quad n=(\psi_{n,S})_*\tfrac{\partial}{\partial u},\quad (\psi_{n,S})^*\tilde{h}=h_S(y)dy^2,\end{aligned} \tag{13.20}$$

where $h_S(y)dy^2$ is a Riemannian metric on S, independent on u. We have $\psi^{-1}_{n,S}(S')=\{(u,y):u=f(y)\}$ for some $f\in C^\infty(S)$ and

$$\psi^{-1}_{n,S'}\circ\psi_{n,S}(u,y)=(u-f(y),\phi_{S'\leftarrow S}(y)),\quad (u,y)\in\mathbb{R}_u\times S. \tag{13.21}$$

Since $\mathscr{I}^-$ is diffeomorphic to $\mathbb{R}\times\mathbb{S}^2$, S is diffeomorphic to $\mathbb{S}^2$. Let m_S denote the unique Riemannian metric on S of constant Gaussian curvature equal to 1. By uniqueness, we have $m_S=(\phi_{S'\leftarrow S})^*m_{S'}$.

DEFINITION 13.5.4. *A conformal frame* $(\tilde{h},n)$ *is a* Bondi frame *if for some* (*and hence for all*) *surface* S *transverse to* n *one has* $\tilde{h}\restriction_S=m_S$.

LEMMA 13.5.5. *The set* $\mathcal{C}$ *of conformal frames contains a unique Bondi frame* $(\tilde{h}_B,n_B)$.

Proof. Let us fix $(\tilde{h},n)\in\mathcal{C}$ and S transverse to n. After transportation by $\psi_{n,S}$, all conformal frames are of the form $(\omega_S^2 h_S,\omega_S^{-1}\partial_u)$ for some $\omega_S\in C^\infty(S)$, $\omega_S>0$. It is well known that any Riemannian metric on $\mathbb{S}^2$ is conformal to the standard metric. This means that there is a unique such ω_S with $\omega_S^2 h_S=m_S$. □

If we fix a transverse surface S and identify S with $\mathbb{S}^2$ we can introduce the so-called *Bondi coordinates* on $\mathscr{I}^-$, (u,θ,φ), such that $n_B=\partial_u$ and $\tilde{h}_B=d\theta^2+\sin^2\theta d\varphi^2$.

The existence of a unique Bondi frame implies the following *rigidity* result: we saw that there exists a diffeomorphism $\psi : \mathscr{I}^- \to \mathbb{R}_u \times \mathbb{S}^2$ such that the natural image of $\mathcal{C}$ under ψ is the set of pairs $(\omega^2 m_{\mathbb{S}^2}, \omega^{-1}\partial_u)$ for $\omega > 0$ an arbitrary smooth function on $\mathbb{S}^2$.This implies that if (M_i, g_i) $i = 1, 2$, are two asymptotically flat spacetimes, there exists a diffeomorphism $\psi : \mathscr{I}_1^- \to \mathscr{I}_2^-$ such that $\psi(\mathcal{C}_1) = \mathcal{C}_2$. Another illustration of this rigidity is the fact that the BMS group defined below is independent of the asymptotically flat spacetime (M, g).

13.5.3. The BMS **group.** We now recall the definition of the *Bondi-Metzner-Sachs group*, see e.g. [**W1**, Section 11] or [**DMP1**]. Its physical interpretation is the group of asymptotic symmetries of (M, g) near past null infinity. If $\chi : \mathscr{I}^- \to \mathscr{I}^-$ is a diffeomorphism, we let χ act on $(\tilde{h}, n)$ by

$$\alpha_\chi(\tilde{h}, n) := ((\chi^{-1})^* \tilde{h}, \chi_* n).$$

Definition 13.5.6. *The* BMS group G_{BMS} *is the group of diffeomorphisms* $\chi : \mathscr{I}^- \to \mathscr{I}^-$ *such that* $\alpha_\chi(\mathcal{C}) \subset \mathcal{C}$.

One can associate to $\chi \in G_{\mathrm{BMS}}$ a conformal factor ω_χ by the rule

$$\alpha_\chi(\tilde{h}_B, n_B) =: (\omega_\chi^2 (\chi^{-1})^* \tilde{h}_B, \omega_\chi^{-1} \chi_* n_B), \tag{13.22}$$

where $(\tilde{h}_B, n_B)$ is the Bondi frame. From $\alpha_{\chi_1} \circ \alpha_{\chi_2} = \alpha_{\chi_1 \circ \chi_2}$ we obtain the identity

$$\omega_{\chi_1 \circ \chi_2} = (\omega_{\chi_1} \circ \chi_2)\omega_{\chi_2}. \tag{13.23}$$

It is convenient to describe the action of the BMS group in Bondi coordinates (u, θ, φ) on $\mathscr{I}^-$ associated to the Bondi frame.

Let us identify $\mathbb{S}^2$ with $\mathbb{C}$ by stereographic projection: $(\theta, \varphi) \mapsto z = \mathrm{e}^{\mathrm{i}\varphi} \coth(\frac{\theta}{2})$, so that $d\theta^2 + \sin^2\theta d\varphi^2 = 4(1 + z\overline{z})^{-2} dz d\overline{z}$.

Functions on $\mathbb{C}$ will be denoted by $f(z, \overline{z})$, to emphasize the fact that they do not need to be holomorphic (nor anti-holomorphic). One can prove that G_{BMS} can be identified with the semi-direct product of $SO^\uparrow(1, 3)$ and $C^\infty(\mathbb{S}^2)$ as follows, see [**DMP1**]:

Let $\Pi : SL(2, \mathbb{C}) \to SO^\uparrow(1, 3)$ be the covering map with $\Pi^{-1}(\mathbb{1}) = \{\pm\mathbb{1}\}$. For $\Lambda = \Pi \begin{pmatrix} a_\Lambda & b_\Lambda \\ c_\Lambda & d_\Lambda \end{pmatrix}$ one sets

$$K_\Lambda(z, \overline{z}) = \frac{1 + |z|^2}{|a_\Lambda z + b_\Lambda|^2 + |c_\Lambda z + d_\Lambda|^2}$$

and one associates to $(\Lambda, f) \in SO^\uparrow(1, 3) \times C^\infty(\mathbb{S}^2)$ the map: $\chi : \mathscr{I}^- \to \mathscr{I}^-$ given in the Bondi coordinates fixed above by the rule

$$(u, z, \overline{z}) \longmapsto (u', z', \overline{z}'),$$

where

$$u' = K_\Lambda(z, \overline{z})(u + f(z, \overline{z})) \quad \text{and} \quad z' = \frac{a_\Lambda z + b_\Lambda}{c_\Lambda z + d_\Lambda}. \tag{13.24}$$

We have

$$\omega_\chi(z, \overline{z}) = K_\Lambda(z, \overline{z})^{-1}. \tag{13.25}$$

The diffeomorphisms obtained for $\Lambda = \mathbb{1}$ are called *supertranslations*.

13.6. The canonical symplectic space on $\mathscr{I}^-$

Assume that (M,g) and $(\tilde{M},\tilde{g})$ (and hence $(M,\tilde{g})$) are globally hyperbolic and the inclusion $i:(M,\tilde{g})\to(\tilde{M},\tilde{g})$ is causally compatible, see Subsection 5.2.6. Let $P=-\Box_g+\frac{1}{6}\mathrm{Scal}_g$, resp. $\tilde{P}$, be the conformal wave operator on (M,g), resp. $(\tilde{M},\tilde{g})$. By Proposition 6.3.1, the map

$$(\mathrm{Sol}_{\mathrm{sc}}(P),q)\ni\phi\longmapsto\tilde{\phi}=\Omega^{-1}\phi\in\mathrm{Sol}_{\mathrm{sc}}(\tilde{P},\tilde{q})$$

is an injective homomorphism of pseudo-Hermitian spaces, and we can consider

$$v:=\tilde{\phi}\restriction_{\mathscr{I}^-}\in C^\infty(\mathscr{I}^-).$$

Since an element χ of the BMS group corresponds to a change $\Omega\to\Omega'=\omega_\chi\Omega$, we see that the natural action of $\chi\in G_{\mathrm{BMS}}$ on functions on $\mathscr{I}^-$ is

$$U_\chi v:=(\omega_\chi v)\circ\chi^{-1}, \tag{13.26}$$

and by (13.23) $G_{\mathrm{BMS}}\ni\chi\mapsto U_\chi\in L(C^\infty(\mathscr{I}^-))$ is a group homomorphism.

In analogy with Proposition 13.2.1, one can now equip suitable subspaces of $C^\infty(\mathscr{I}^-)$, such as, for example, $C_0^\infty(\mathscr{I}^-)$, with a canonical Hermitian form. Let $(\tilde{h}_B,n_B)$ be the Bondi frame and S be transverse to n_B.

Definition 13.6.1. *We set for $v_1,v_2\in C_0^\infty(\mathscr{I}^-)$*

$$\overline{v}_1\cdot qv_2:=\mathrm{i}\int_{\mathbb{R}\times S}\big(\partial_u\overline{w}_1w_2-\overline{w}_1\partial_uw_2\big)du\,dVol_{m_S},$$

where

$$w=v\circ\psi_{n_B,S}. \tag{13.27}$$

Proposition 13.6.2. (1) *the Hermitian form q is independent on the choice of the transverse surface S,*

(2) *one has $(U_\chi)^*qU_\chi=q$ for $\chi\in G_{\mathrm{BMS}}$, i.e. G_{BMS} acts as unitary transformations of $(C_0^\infty(\mathscr{I}^+),q)$.*

Proof. Let us first prove (1). If S' is another tranverse surface and $w'=v\circ\psi_{n_B,S'}$, then from (13.21) it follows that

$$w'_j(u',y')=w_j(u'+f'(y'),\phi_{S\leftarrow S'}(y')), \tag{13.28}$$

and $(\phi_{S\leftarrow S'})^*m_{S'}=m_S$, which implies (1).

To prove (2), we work again with the Bondi frame $(\tilde{h}_B,n_B)$, and identify $\mathscr{I}^-$ with $\mathbb{R}\times S$ using $\psi_{n_B,S}$ and S with $\mathbb{C}$ as in Subsection 13.5.3. The charge q takes the form

$$\overline{v}_1\cdot qv_2=\mathrm{i}\int_{\mathbb{R}\times\mathbb{C}}\big(\partial_u\overline{w}_1w_2-\overline{w}_1\partial_uw_2\big)\frac{4}{(1+z\overline{z})^2}dudzd\overline{z}.$$

We equip $\mathbb{R}\times\mathbb{C}$ with the density $4(1+|z|^2)^{-2}dudzd\overline{z}$ and denote by $w\mapsto V_\chi w$ the action of $\chi\in G_{\mathrm{BMS}}$ obtained from U_χ and the identification (13.27). The operator $D_u=\mathrm{i}^{-1}\partial_u$ is essentially selfadjoint on $C_0^\infty(\mathbb{R}\times\mathbb{C})$, and integrating by parts we obtain that

$$\overline{v}_1\cdot qv_2=2(w_1|D_uw_2)_{L^2(\mathbb{R}\times\mathbb{C})}.$$

From (13.24) it follows, by an easy computation, that

$$V_\chi^*V_\chi=K_\Lambda\mathbb{1},\ V_\chi^*D_uV_\chi=D_u, \tag{13.29}$$

where we consider V_χ as an operator on $L^2(\mathbb{R}\times\mathbb{C})$ and K_Λ is the operator of multiplication by $K_\Lambda(z,\overline{z})$. This implies (2). □

There is a considerable freedom in the choice of a symplectic space $\mathcal{Y}$ on which q is defined.

A natural canonical choice is the space $H^1(\mathscr{I}^-)$ defined as the completion of $C_0^\infty(\mathscr{I}^-)$ with respect to the norm

$$\|v\|_1^2 = \|w\|^2_{L^2(\mathbb{R}\times S)} + \|\partial_u w\|^2_{L^2(\mathbb{R}\times S)},$$

where as above $w = v \circ \psi_{n_B,S}$ and $\mathbb{R}\times S$ is equipped with the density $du\, dVol_{m_S}$.

The operator $D_u = \mathrm{i}^{-1}\partial_u$ acting on $L^2(\mathbb{R}\times S)$ is essentially selfadjoint on $C_0^\infty(\mathbb{R}\times S)$ and $H^1(\mathscr{I}^-)$ is the inverse image of $\operatorname{Dom} D_u$ under the map $v \mapsto w = v \circ \psi_{n_B,S}$.

A change of transverse surface S does not change the space $H^1(\mathscr{I}^-)$, but simply equips it with an equivalent norm. The group G_{BMS} acts on $(H^1(\mathscr{I}^-), q)$ by bounded unitary transformations and q is non-degenerate on $H^1(\mathscr{I}^-)$, since D_u is injective.

13.6.1. The canonical quasi-free state on $\mathscr{I}^-$. We now describe the construction of a canonical quasi-free state $\omega_{\mathscr{I}^-}$ on $\mathrm{CCR}^{\mathrm{pol}}(H^1(\mathscr{I}^-), q)$, due to Moretti [**Mo1**].

Proposition 13.6.3. *Let us set*

$$\overline{v}_1 \cdot \Lambda^\pm v_2 := 2(w_1 | \mathbb{1}_{\mathbb{R}^\pm}(D_u)|D_u| w_2)_{L^2(\mathbb{R}\times S)}, \quad v_i \in H^1(\mathscr{I}^-),$$

for $w_i = v_i \circ \psi_{n_B,S}$. Then

(1) *$\Lambda^\pm$ are independent of the choice of the transverse surface S,*
(2) *$\Lambda^\pm$ are the covariances of a pure, quasi-free state $\omega_{\mathscr{I}^-}$ on $\mathrm{CCR}^{\mathrm{pol}}(H^1(\mathscr{I}^-), q)$ which is invariant under the action of G_{BMS}.*

Proof. If S, S' are two transverse surfaces and $w = v \circ \psi_{n_B,S}$, $w' = v \circ \psi_{n_B,S'}$, then $w' = U_{S'\leftarrow S} w$, where $U_{S'\leftarrow S}$ is given in (13.28). We check that $U_{S'\leftarrow S} : L^2(\mathbb{R}\times S) \to L^2(\mathbb{R}\times S')$ is unitary with $U_{S'\leftarrow S} D_u U^*_{S'\leftarrow S} = D_u$. This implies that $\Lambda^\pm$ are independent of the choice of S.

To prove (2), we use the notation in the proof of Proposition 13.6.2. Let $S_\chi = V_\chi K_\Lambda^{-\frac{1}{2}}$, which is unitary by (13.29). Since K_Λ commutes with D_u we have $S^*_\Lambda D_u S_\Lambda = D_u$, hence $S^*_\Lambda \mathbb{1}_{\mathbb{R}^\pm}(D_u)|D_u|S_\Lambda = \mathbb{1}_{\mathbb{R}^\pm}(D_u)|D_u|$ by functional calculus. Using again the fact that K_Λ commutes with D_u, this implies that $V^*_\Lambda \mathbb{1}_{\mathbb{R}^\pm}(D_u)|D_u|V_\Lambda = \mathbb{1}_{\mathbb{R}^\pm}(D_u)|D_u|$, i.e. that $U^*_\chi \Lambda^\pm U_\chi = \Lambda^\pm$. □

Moretti proved in [**Mo1**] that $\omega_{\mathscr{I}^-}$ is the *unique* pure quasi-free state ω on $\mathrm{CCR}^{\mathrm{pol}}(H^1(\mathscr{I}^-), q)$ with the following two properties:

(1) ω is invariant under G_{BMS},
(2) if $\{T_s\}_{s\in\mathbb{R}} \subset G_{\mathrm{BMS}}$ is the one-parameter subgroup of translations in u and $\alpha_s = U_{T_s}$, then ω is a *non-degenerate ground state* for $\{\alpha_s\}_{s\in\mathbb{R}}$, see Definition 9.1.1.

13.6.2. Construction of a quasi-free state in M. To obtain quasi-free states for P in M from states on $\mathrm{CCR}^{\mathrm{pol}}(H^1(\mathscr{I}^-), q)$, $\varrho_{\mathscr{I}^-}\mathrm{Sol}_{\mathrm{sc}}(P)$ should be contained in $H^1(\mathscr{I}^-)$ for $\varrho_{\mathscr{I}^-}\phi = (\Omega^{-1}\phi)\restriction_{\mathscr{I}^-}$.

If we introduce coordinates (u, y) on $\mathscr{I}^-$ as in Subsection 13.5.2, then it follows from Definition 13.5.1 (3) that $J^{\tilde{M}}(K) \cap \mathscr{I}^-$ is included in $\psi^{-1}_{n,S}(\{u \le C_K\})$ for any $K \Subset M$, so the support of $\varrho_{\mathscr{I}^-}\phi$ for $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$ only extends towards $-\infty$ in the u variable.

If (M, g) is asymptotically flat with *past time infinity*, see [**Mo2**, Appendix A] for a precise definition, then $u = -\infty$ corresponds to an actual point i^- of $\tilde{M}$, and the situation is essentially the same as the one in Section 13.1, i.e. (M, g) is modulo a conformal transformation the interior of a smooth, future lightcone.

In more complicated situations, like the Schwarzschild spacetime, see [**DMP3**] or cosmological spacetimes, see [**DMP4**], it is necessary to prove some decay estimates of $\varrho_{\mathscr{I}^-}\phi$ and its derivative in u when $u \to -\infty$ to ensure that $\varrho_{\mathscr{I}^-}\mathrm{Sol}_{\mathrm{sc}}(P) \subset H^1(\mathscr{I}^-)$. The discussion of these estimates is beyond the scope of this survey.

CHAPTER 14

Klein-Gordon fields on spacetimes with Killing horizons

As recalled in the Introduction, one of the most spectacular results of QFT on curved spacetimes is the Hawking effect, discovered by Hawking [**Ha**]. Hawking considered a Klein-Gordon field in a spacetime describing the formation of a black hole by gravitational collapse of a spherically symmetric star, the spacetime being eventually equal to the *Schwarzschild* spacetime in the exterior of the black hole horizon. Considering the state which in the past is the vacuum state for the region outside of the star, he gave some heuristic arguments to show that in the far future and far away from the horizon this state is a thermal state at *Hawking temperature* $T_{\rm H} = \kappa(2\pi)^{-1}$.

The first complete justification of the Hawking effect is due to Bachelot [**B**], who considered the same situation as Hawking.

Another derivation of the Hawking effect is due to Fredenhagen and Haag [**FH**]. They considered the same situation as Hawking and the more general case of a state for the Klein-Gordon field whose two-point function is assumed to be asymptotic to that of the vacuum at spatial infinity and of Hadamard form near the horizon.

We discuss in this chapter another phenomenon related to the Hawking radiation, namely, the existence of a 'vacuum state' for a Klein-Gordon field on spacetimes with a *bifurcate Killing horizon*, see Section 14.1 for a precise definition. The existence of such a state is related to the so-called *Unruh effect*, [**U**], which we now briefly describe.

In the Minkowski spacetime $(\mathbb{R}^{1,d}, \eta)$ one considers a *right wedge* $\mathcal{M}^+ = \{(t, \mathrm{x}) : |t| < \mathrm{x}_1\}$, where x_1 is a space coordinate. The spacetime $(\mathcal{M}^+, \eta)$ is invariant under the Lorentz boosts with generator

$$X = a(\mathrm{x}_1\partial_t + t\partial_{\mathrm{x}_1}),$$

where $a > 0$ is an arbitrary constant. Although X is not globally time-like in $\mathbb{R}^{1,d}$, it is time-like in $\mathcal{M}^+$ and its integral curves in $\mathcal{M}^+$ are worldlines of uniformly accelerated observers, with acceleration equal to a.

Since X is time-like in $\mathcal{M}^+$, one can construct, for any $\beta > 0$, the associated β-KMS state ω_β for the Klein-Gordon operator $-\Box + m^2$ restricted to $\mathcal{M}^+$, see Chapter 9. Unruh proved that if $\beta = (2\pi)a^{-1}$, then ω_β is the restriction to $\mathcal{M}^+$ of the Minkowski vacuum $\omega_{\rm vac}$. This result is interpreted as the fact that the Minkowski vacuum state is seen by uniformly accelerated observers with acceleration a as a thermal state at temperature $a(2\pi)^{-1}$.

Note that the Killing vector field X vanishes at $\mathcal{B} = \{t = \mathrm{x}_1 = 0\}$, which is the intersection of the two null hyperplanes $\{t = \pm\mathrm{x}_1\}$, whose union is an example of a bifurcate Killing horizon. In spacetimes with a bifurcate Killing horizon, the existence of a state analogous to the Minkowski vacuum, called the *Hartle-Hawking-Israel state*, was conjectured by Hartle and Hawking [**HH**] and Israel [**Is**], using formal Wick rotation arguments.

We will explain the rigorous construction of the HHI state in [**G2**], which is based on methods already used in Chapter 12, namely the *Calderón projectors* from the theory of elliptic boundary value problems.

For *static* Killing horizons, i.e. when X is orthogonal to some Cauchy surface in the exterior region, the HHI state was already constructed by Sanders in [**S3**].

The condition that the Killing vector field X generating the horizon is time-like in the exterior region excludes the physically important *Kerr* spacetime. In fact, applying Proposition 9.2.1 to the exterior region of the Kerr spacetime, we know that no KMS state for X exists in the exterior region.

Much more general non-existence results on the Kerr spacetime were shown by Kay and Wald in [**KW**]. For example assuming the existence of some solutions of the Klein-Gordon equation exhibiting *superradiance*, it is shown in [**KW**] that there exist no X-invariant state which is Hadamard near the horizon. Therefore, it is expected that no HHI state exists in the Kerr spacetime.

14.1. Spacetimes with bifurcate Killing horizons

Let (M, g) be a globally hyperbolic spacetime with a complete Killing vector field X. We assume that $\mathcal{B} := \{x \in M : X(x) = 0\}$ is a compact, connected submanifold of codimension 2, called the *bifurcation surface*. If moreover there exists a smooth, space-like Cauchy surface Σ containing $\mathcal{B}$, the triple (M, g, X) is called a *spacetime with a bifurcate Killing horizon*, see [**KW**, Section 2]. If N, w are the lapse function and shift vector field associated to X, Σ as in Section 9.2, the Cauchy surface Σ splits as

$$\Sigma = \Sigma^- \cup \mathcal{B} \cup \Sigma^+, \quad \Sigma^\pm := \{y \in \Sigma : \pm N(y) > 0\},$$

i.e. X is future/past directed on $\Sigma^\pm$. Accordingly one can split M as

$$M = \mathcal{M}^+ \cup \mathcal{M}^- \cup \overline{\mathcal{F}} \cup \overline{\mathcal{P}},$$

where the *future cone* $\mathcal{F} := I^+(\mathcal{B})$, *the past cone* $\mathcal{P} := I^-(\mathcal{B})$, and the *right/left wedges* $\mathcal{M}^\pm := D(\Sigma^\pm)$, are all globally hyperbolic when equipped with g.

The boundary of the future cone $\partial\mathcal{F}$ may be a black hole horizon, in which case $\partial\mathcal{P}$ is the corresponding white hole horizon. The *bifurcate Killing horizon* is

$$\mathcal{H} := \partial\mathcal{F} \cup \partial\mathcal{P},$$

and the Killing vector field X is tangent to $\mathcal{H}$. In Fig. 7 below the vector field X is represented by arrows.

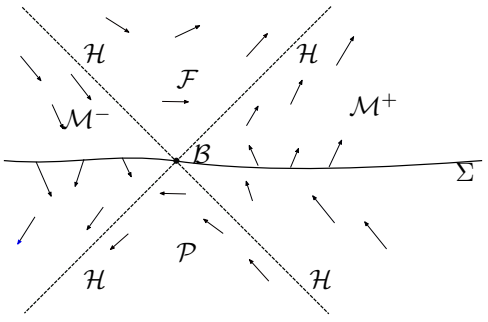


Fig. 7

14.1.1. The surface gravity. An important quantity associated to the Killing horizon $\mathcal{H}$ is its *surface gravity*, defined by

$$\kappa^2 = -\frac{1}{2}(\nabla^b X^a \nabla_b X_a)|_{\mathcal{B}}, \quad \kappa > 0.$$

It is a fundamental fact, see [**KW**, Section 2], that the scalar κ is constant on $\mathcal{B}$ and actually on the whole horizon $\mathcal{H}$.

14.1.2. Wedge reflection. In concrete situations, like the Schwarzschild or Kerr spacetimes, the metric g is originally defined only on the right wedge $\mathcal{M}^+$ and first extended to the future cone $\mathcal{F}$ by a new choice of coordinates. The regions $\mathcal{P}$, $\mathcal{M}^-$ are constructed as copies of $\mathcal{F}$, $\mathcal{M}^+$, with reversed time orientation, glued together along $\mathcal{B}$. This motivates one to assume the existence of a *wedge reflection*, i.e. an isometric involution R of $\mathcal{M}^- \cup U \cup \mathcal{M}^+$, where U is a neighborhood of $\mathcal{B}$ in M, such that R reverses the time orientation, $R = Id$ on $\mathcal{B}$ and $R^* X = X$.

It can be shown, see [**S3**], that there exists a smooth, space-like Cauchy surface Σ with $\mathcal{B} \subset \Sigma$ such that $R : \Sigma \xrightarrow{\sim} \Sigma$. The restriction r of R to Σ is called a *weak wedge reflection*. We have

$$r|_{\mathcal{B}} = Id, \quad r : \Sigma^{\pm} \xrightarrow{\sim} \Sigma^{\mp}. \tag{14.1}$$

In the sequel we will fix such a Cauchy surface.

14.1.3. Stationary Killing horizons. The bifurcate Killing horizon $\mathcal{H}$ is called *stationary*, resp. *static*, if the Killing vector field X is time-like in $\mathcal{M}^+$, resp. time-like and orthogonal to Σ in $\mathcal{M}^+$.

14.2. Klein-Gordon fields

Let us consider a Klein-Gordon operator

$$P = -\Box_g + V,$$

where $V \in C^\infty(M; \mathbb{R})$ has the same invariance properties as g, i.e. $X \cdot V = 0$, $V \circ R = V$. We also strengthen the condition $V > 0$ in Section 9.3 to

$$V(x) \geq m^2, \quad x \in M, \ m > 0,$$

i.e. we restrict our attention to massive Klein-Gordon fields.

If X is time-like in $\mathcal{M}^+$, we can apply Sections 9.3, Subsection 9.5 to the Klein-Gordon operator P , on the globally hyperbolic spacetime $(\mathcal{M}^+, g)$, with Cauchy surface Σ^+. We obtain, for each $\beta > 0$ the β-KMS state ω_β acting on $\mathrm{CCR}^{\mathrm{pol}}(C_0^\infty(\Sigma^+; \mathbb{C}^2), q)$.

Following Section 4.8, we can associate to ω_β the *doubled* state ω_{d}, which is associated to the doubled Hermitian space

$$(C_0^\infty(\Sigma^+; \mathbb{C}^2) \oplus C_0^\infty(\Sigma^+; \mathbb{C}^2), q \oplus -q). \tag{14.2}$$

14.3. Wick rotation

The key step in the construction of the Hartle-Hawking state is the interpretation of the double β-KMS state ω_{D} using the Wick rotation in Killing time coordinates. We will now explain this important step.

14.3.1. The Wick rotated metric. As in Section 9.2, we can identify $\mathcal{M}^+$ with $\mathbb{R}\times\Sigma^+$, the metric g taking the form

$$g=-N^2(y)dt^2+h_{ij}(y)(dy^i+w^i(y)dt)(dy^j+w^j(y)dt),$$

see (9.12). As in Chapter 12, we can perform the *Wick rotation*, replacing the Killing time coordinate t by is. In this way we obtain from g the *complex metric*

$$g^{\rm eucl}=N^2(y)ds^2+h_{ij}(y)\big(dy^i+\mathrm{i}w^i(y)ds\big)\big(dy^j+\mathrm{i}w^j(y)ds\big).$$

If $\xi=(\tau,\eta)\in\mathbb{C}T_yM$ and $y\in\Sigma^+$, then

$$\begin{aligned}\overline{\xi}\cdot g^{\rm eucl}(y)\xi=\;&(N^2(y)-w(y)\cdot h(y)w(y))\overline{\tau}\tau+\overline{\eta}\cdot h(y)\eta\\&+\mathrm{i}(w(y)\cdot h(y)\overline{\eta}\tau+\overline{\tau}w(y)\cdot h(y)\eta).\end{aligned}$$

Since $X=\frac{\partial}{\partial t}$ is time-like in $\mathcal{M}^+$, we know that $N^2(y)>w^i(y)h_{ij}(y)w^j(y)$, from which we deduce that

$$|\mathrm{Im}(\overline{\xi}\cdot g^{\rm eucl}(y)\xi)|\leq c(y)\mathrm{Re}(\overline{\xi}\cdot g^{\rm eucl}(y)\xi),\quad y\in\Sigma^+, \tag{14.3}$$

for some $c(y)>0$. It is convenient to have some uniformity in y in the inequality (14.3), which follows if we require that there exists $\delta>0$ such that

$$X(y)+\delta w(y)\;\text{ is time-like for } y\in\Sigma. \tag{14.4}$$

One can show that it suffices to assume that (14.4) holds away from a compact neighborhood of $\mathcal{B}$ in Σ, i.e. near spatial infinity. From (14.4) we deduce the uniform version of (14.3), namely, there exists $c>0$ such that

$$|\mathrm{Im}(\overline{\xi}\cdot g^{\rm eucl}(y)\xi)|\leq c\mathrm{Re}(\overline{\xi}\cdot g^{\rm eucl}(y)\xi),\quad y\in\Sigma^+. \tag{14.5}$$

Another useful fact is that $|g^{\rm eucl}|(y)=|\det g^{\rm eucl}(y)|=N^2(y)|h(y])>0$ for all $y\in\Sigma$, so the density $dVol_{g^{\rm eucl}}=|g^{\rm eucl}|^{\frac{1}{2}}dsdy$ is positive.

14.3.2. The Wick rotated operator. The Klein-Gordon operator P takes the form

$$P=(\partial_t+w^*)N^{-2}(\partial_t+w)+h_0,$$

see (9.17), and becomes after Wick rotation the differential operator

$$P^{\rm eucl}=(-\partial_s+\mathrm{i}w^*)N^{-2}(\partial_s+\mathrm{i}w)+h_0.$$

One can define the Laplace-Beltrami operator $\Delta_{g^{\rm eucl}}$ associated to the complex metric $g^{\rm eucl}$ as in the Riemannian case and one has $P^{\rm eucl}=-\Delta_{g^{\rm eucl}}+V(y)$. It also follows from (14.5) that $P^{\rm eucl}$ is an elliptic differential operator.

Let us now associate to $P^{\rm eucl}$ some densely defined operator. It is a well-known fact that to describe quantum fields at temperature β^{-1} by Euclidean methods, the Euclidean time s should belong to the circle $\mathbb{S}_\beta$ of length β.

Therefore, we set $M^{\rm eucl}:=\mathbb{S}_\beta\times\Sigma^+$ and consider the sesquilinear form

$$Q_\beta(u,u)=\int_{M^{\rm eucl}}\overline{u}P^{\rm eucl}u\,dVol_{g^{\rm eucl}},\quad \mathrm{Dom}\,Q_\beta=C_0^\infty(M^{\rm eucl}).$$

It follows from (14.5) that Q_β is *sectorial*, i.e.,

$$|\mathrm{Im}\,Q_\beta(u,u)|\leq c\mathrm{Re}\,Q_\beta(u,u),\quad u\in\mathrm{Dom}\,Q_\beta,$$

and hence closeable. The domain of its closure $Q_\beta^{\rm cl}$ equals the Sobolev space $H^1(M^{\rm eucl})$, defined as the completion of $C_0^\infty(M^{\rm eucl})$ with respect to the norm

$$\|u\|_1^2=\int_{M^{\rm eucl}}\big(\nabla\overline{u}\cdot\mathrm{Re}(g^{\rm eucl})^{-1}(y)\nabla u+V(y)\overline{u}u\big)dVol_{g^{\rm eucl}}.$$

By the Lax-Milgram theorem, one associates to $Q_\beta^{\rm cl}$ a boundedly invertible operator

$$P_\beta^{\rm eucl}:H^1(M^{\rm eucl})\xrightarrow{\sim}H^1(M^{\rm eucl})^*,$$

which corresponds to imposing β-periodic boundary conditions for the operator P^{eucl}.

14.3.3. Calderón projectors. Consider the open set

$$\Omega :=]0, \beta/2[\times \Sigma^+ \subset M^{\mathrm{eucl}}.$$

Note that $\partial\Omega$ has two connected components $\{0\} \times \Sigma^+$ and $\{\beta/2\} \times \Sigma^+$, both identified with Σ^+. We will use the notation introduced in Section 12.7 for spaces of distributions on Ω.

One defines the *outer unit normal* to $\partial\Omega$ for the complex metric g^{eucl} as the unique complex vector field ν such that

$$\text{(i)} \quad \nu(x) \cdot g^{\mathrm{eucl}}(x) v = 0, \ \forall v \in T_x \partial\Omega,$$

$$\text{(ii)} \quad \nu(x) \cdot g^{\mathrm{eucl}}(x) \nu(x) = 1,$$

$$\text{(iii)} \quad \mathrm{Re}\, \nu(x) \text{ is outwards pointing.}$$

We see that ν equals $-N^{-1}(\frac{\partial}{\partial s} - \mathrm{i}w)$ on $\{0\} \times \Sigma^+$ and its opposite on $\{\beta/2\} \times \Sigma^+$.

One can then define the trace

$$\gamma u = \begin{pmatrix} u\restriction_{\partial\Omega} \\ \nu \cdot \nabla u\restriction_{\partial\Omega} \end{pmatrix} \in C^\infty(\partial\Omega; \mathbb{C}^2)$$

for $u \in \overline{C^\infty}(\Omega)$ with $P^{\mathrm{eucl}} u = 0$ in Ω and the Calderón projectors $c_\beta^\pm$ associated to $(P_\beta^{\mathrm{eucl}}, \Omega)$ as in Section 12.7, see [**G2**, Subsection 8.7] for the precise definitions. The important observation now is that the doubled state ω_{d} constructed from ω_β can be expressed in terms of the Calderón projectors $c_\beta^\pm$. In fact one has, see [**G2**, Proposition 8.8]:

Proposition 14.3.1. *The covariances of ω_{d} are equal to*

$$\lambda_{\mathrm{d}}^\pm = \pm Q \circ (\mathbb{1} \oplus T)^{-1} c_\beta^\pm (\mathbb{1} \oplus T), \quad Q = q \oplus q,$$

where $T = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$.

Two comments are in order at this point. First, the Calderón projectors $c_\beta^\pm$ are defined on $C_0^\infty(\partial\Omega; \mathbb{C}^2)$, or equivalently on $C_0^\infty(\Sigma^+; \mathbb{C}^2) \oplus C_0^\infty(\Sigma^+; \mathbb{C}^2)$, which is exactly the doubled phase space on which the doubled state ω_{d} is defined.

Second the operator T takes care of the fact that ω_{d} is associated to the Hermitian form $q \oplus -q$, see (14.2), and not $Q = q \oplus q$.

14.4. The double β-KMS state in $\mathcal{M}^+ \cup \mathcal{M}^-$

Recall that the wedge reflection R maps $\mathcal{M}^+$ to $\mathcal{M}^-$ and reverses the time orientation. It is hence easy to obtain from ω_{d} a pure quasi-free state ω_{D} in $\mathcal{M}^+ \cup \mathcal{M}^-$, called the *double* β-KMS *state*. This provides a first extension of the thermal state ω_β in $\mathcal{M}^+$ to a pure state in $\mathcal{M}^+ \cup \mathcal{M}^-$. The Cauchy surface covariances $\lambda_{\mathrm{D}}^\pm$ of ω_{D} are the sesquilinear forms on $(C_0^\infty(\Sigma^+; \mathbb{C}^2), q) \oplus (C_0^\infty(\Sigma^-; \mathbb{C}^2), q)$ given by

$$\lambda_{\mathrm{D}}^\pm = \pm Q \circ (\mathbb{1} \oplus r^*)^{-1} c_\beta^\pm (\mathbb{1} \oplus r^*),$$

where $r^* f(y) = f(r(y))$. Note that

$$\mathcal{R}_\Sigma = T r^* : (C_0^\infty(\Sigma^-; \mathbb{C}^2), q) \xrightarrow{\sim} (C_0^\infty(\Sigma^+; \mathbb{C}^2), -q).$$

is exactly the unitary map on Cauchy data induced by the wedge reflection $R : C_0^\infty(\mathcal{M}^+) \xrightarrow{\sim} C_0^\infty(\mathcal{M}^-)$.

14.5. The extended Euclidean metric and the Hawking temperature

The constructions carried out up to now are valid for any $\beta > 0$. The Euclidean metric $g^{\rm eucl}$ usually degenerates at the bifurcation surface $\mathcal{B}$. In fact, for $\omega \in \mathcal{B}$, let n_ω the unit normal to $\mathcal{B}$ for the induced metric h on Σ, pointing towards Σ^+. Using n_ω one can introduce Gaussian normal coordinates (u, ω) on a neighborhood of $\mathcal{B}$ in Σ, with Σ^+ corresponding to $u > 0$. One can then show that in the coordinates (s, u, ω), the Euclidean metric $g^{\rm eucl}$ near $u = 0$ takes the form

$$\kappa^2 u^2 ds^2 + du^2 + k(\omega) d\omega^2,$$

modulo higher-order terms depending only on (u^2, ω), where the Riemannian metric $k(\omega)d\omega^2$ is the restriction of $h(y)dy^2$ to $\mathcal{B}$, see [**G2**, App. A].

We recognize in the first two terms the expression of the flat Riemannian metric $dX^2 + dY^2$, if $X = u\cos(\kappa s)$, $Y = u\sin(\kappa s)$, i.e. if (u, s) are polar coordinates.

Since $s \in \mathbb{S}_\beta$, we see that if $\beta = (2\pi)\kappa^{-1}$, i.e. if β^{-1} equals the *Hawking temperature* $\kappa(2\pi)^{-1}$, then $g^{\rm eucl}$ extends across $\mathcal{B}$ to a smooth complex metric $g^{\rm eucl}_{\rm ext}$, living on a smooth manifold $M^{\rm eucl}_{\rm ext}$, which near $\mathcal{B}$ is diffeomorphic to $\mathbb{R}^2 \times \mathcal{B}$. For other values of β, no such smooth extension exists, and $g^{\rm eucl}$ has a conical singularity at $\mathcal{B}$.

It is also important to understand the open set $\Omega_{\rm ext} \subset M^{\rm eucl}_{\rm ext}$ corresponding to $\Omega \subset M^{\rm eucl}$. Its boundary $\partial\Omega_{\rm ext}$ is obtained by gluing together along $\mathcal{B}$ the two connected components $\{0\} \times \Sigma^+$ and $\{\beta/2\} \times \Sigma^+$ of $\partial\Omega$. Actually, $\partial\Omega_{\rm ext}$ is diffeomorphic to Σ. The reason for this is that in coordinates (u, ω), the weak wedge reflection r becomes simply the reflection $(u, \omega) \mapsto (-u, \omega)$, and Σ^+ is identified with Σ^- by r.

14.6. The Hartle-Hawking-Israel state

One can associate to the extended metric $g^{\rm eucl}_{\rm ext}$ a Laplace-Beltrami operator $P^{\rm eucl}_{\rm ext}$ and consider its Calderón projectors $c^\pm_{\rm ext}$ for the open set $\Omega_{\rm ext}$.

Since the boundary $\partial\Omega_{\rm ext}$ is diffeomorphic to Σ, it is tempting to use $c^\pm_{\rm ext}$ to construct Cauchy surface covariances on Σ, which, if the required positivity properties are satisfied, will define a quasi-free state on the whole of M. It turns out that this is indeed the case, the resulting state being the sought-for *Hartle-Hawking-Israel state*. Let us thus summarize the main result of [**G2**].

THEOREM 14.6.1. *There exists a state $\omega_{\rm HHI}$ for P in (M, g), called the* Hartle-Hawking-Israel state*, such that:*

(1) *$\omega_{\rm HHI}$ is a pure Hadamard state in M;*
(2) *the restriction of $\omega_{\rm HHI}$ to $\mathcal{M}^+ \cup \mathcal{M}^-$ is the double β-KMS state $\omega_{\rm D}$ at Hawking temperature $T_{\rm H} = \kappa(2\pi)^{-1}$, where κ is the surface gravity of the horizon;*
(3) *$\omega_{\rm HHI}$ is the unique extension of $\omega_{\rm D}$ such that its spacetime covariances $\Lambda^\pm$ map $C^\infty_0(M)$ into $C^\infty(M)$ continuously. In particular, it is the unique Hadamard extension of $\omega_{\rm D}$.*

Proof. Let us now explain some ingredients of the proof of Theorem 14.6.1, which essentially relies on known results on Calderón projectors and Sobolev spaces. We recall that $H^s_{\rm loc}(N)$, resp. $H^s_{\rm c}(N)$ denote the local, resp. compactly supported Sobolev spaces on the manifold N.

Let us first check that $\omega_{\rm HHI}$ is indeed an extension of $\omega_{\rm D}$, i.e., that $\lambda^\pm_{\rm HHI}$ equal $\lambda^\pm_{\rm D}$ on $C^\infty_0(\Sigma \setminus \mathcal{B}; \mathbb{C}^2)$.

The Calderón projectors $c^\pm_{\rm ext}$ are constructed using the inverse of $P^{\rm eucl}_{\rm ext}$, which as for $P^{\rm eucl}$ is constructed from a sesquilinear form $Q_{\rm ext}$. Clearly, $Q_{\rm ext}$ and Q_β coincide on $C^\infty_0(M^{\rm eucl}_{\rm ext} \setminus \mathcal{B})$. Near $\mathcal{B}$ the topology of the domain of the closure of $Q_{\rm ext}$ is the topology of $H^1_{\rm loc}(M^{\rm eucl}_{\rm ext})$. Since $\mathcal{B}$ is of codimension 2 in $M^{\rm eucl}_{\rm ext}$, this

implies that $C_0^\infty(M_{\rm ext}^{\rm eucl}\setminus\mathcal{B})$ is a form core for $Q_{\rm ext}$. This immediately implies that $\lambda^\pm_{\rm HHI}$ and $\lambda^\pm_{\rm D}$ coincide on $C_0^\infty(\Sigma\setminus\mathcal{B};\mathbb{C}^2)$.

From this fact one can also easily deduce that $\lambda^\pm_{\rm HHI}$ are indeed the Cauchy surface covariances of a state, i.e., that

$$\lambda^\pm_{\rm HHI}\geq 0,\ \lambda^+_{\rm HHI}-\lambda^-_{\rm HHI}=q. \tag{14.6}$$

Let us explain this argument: it is known that Calderón projectors for second-order elliptic operators, hence in particular $c^\pm$, are continuous from $H_{\rm c}^{\frac{1}{2}}(\Sigma)\oplus H_{\rm c}^{-\frac{1}{2}}(\Sigma)$ to $H_{\rm loc}^{\frac{1}{2}}(\Sigma)\oplus H_{\rm loc}^{-\frac{1}{2}}(\Sigma)$. From this we deduce immediately that $\lambda^\pm_{\rm HHI}$ are continuous on $H_{\rm c}^{\frac{1}{2}}(\Sigma)\oplus H_{\rm c}^{-\frac{1}{2}}(\Sigma)$.

Since $\mathcal{B}$ is of codimension 1 in Σ, we know that the space $C_0^\infty(\Sigma\setminus\mathcal{B};\mathbb{C}^2)$ is dense in $H_{\rm c}^{\frac{1}{2}}(\Sigma)\oplus H_{\rm c}^{-\frac{1}{2}}(\Sigma)$. The restrictions of $\lambda^\pm_{\rm HHI}$ to $C_0^\infty(\Sigma\setminus\mathcal{B};\mathbb{C}^2)$ equal $\lambda^\pm_{\rm D}$, and so satisfy (14.6), since they are the Cauchy surface covariances of the state $\omega_{\rm D}$. By the above density result, this implies that (14.6) holds on $C_0^\infty(\Sigma;\mathbb{C}^2)$, as claimed. The purity of $\omega_{\rm HHI}$ follows similarly from the purity of $\omega_{\rm D}$.

Further, let us explain how to prove that $\omega_{\rm HHI}$ is a Hadamard state. The restriction of $\omega_{\rm HHI}$ to $\mathcal{M}^+$ is a Hadamard state for P, since it is a $(2\pi)\kappa^{-1}$-KMS state for a time-like, complete Killing vector field. The restriction of $\omega_{\rm HHI}$ to $\mathcal{M}^-$ is also a Hadamard state for P.

This implies that the restriction of $\omega_{\rm HHI}$ to $\mathcal{M}^+\cup\mathcal{M}^-$ is a Hadamard state. The same is true of the restriction of a reference Hadamard state $\omega_{\rm ref}$ in M (see Theorem 11.8.1) to $\mathcal{M}^+\cup\mathcal{M}^-$. Passing to Cauchy surface covariances on $\Sigma^+\cup\Sigma^-$, this implies that if $\chi\in C_0^\infty(\Sigma^\pm)$, then $\chi\circ(\lambda^\pm_{\rm HHI}-\lambda^\pm_{\rm ref})\circ\chi$ is a smoothing operator on Σ. This implies that $\lambda^\pm_{\rm HHI}-\lambda^\pm_{\rm ref}$ is smoothing, which shows that $\omega_{\rm HHI}$ is a Hadamard state.

If fact let a be one of the entries of $\lambda^\pm_{\rm HHI}-\lambda^\pm_{\rm ref}$, which is a scalar pseudodifferential operator belonging to $\Psi^m(\Sigma)$ for some $m\in\mathbb{R}$. We know that $\chi\circ a\circ\chi$ is smoothing for any $\chi\in C_0^\infty(\Sigma\setminus\mathcal{B})$. Then its principal symbol $\sigma_{\rm pr}(a)$ vanishes on $T^*(\Sigma\setminus\mathcal{B})$ hence on $T^*\Sigma$ by continuity, so $a\in\Psi^{m-1}(\Sigma)$. Iterating this argument, we obtain that a is smoothing.

For the proof of the uniqueness statement (3) we refer the reader to **[G2]**. □

CHAPTER 15

Hadamard states and scattering theory

In this chapter we study the construction of Hadamard states from *scattering data*, i.e., from data at future or past *time infinity*. This construction is related to the construction of Hadamard states from past or future null infinity on asymptotically flat spacetimes, which we reviewed in Chapter 13. The geometric assumption on the spacetime (M, g) is that it should be *asymptotically static*, at past or future time infinity, see Section 15.1. Roughly speaking, this means that M should be of the form $\mathbb{R}\times\Sigma$ and g should tend to a standard static metric $g_{\mathrm{out/in}}$, see Subsections 5.3.3, when $t \to \pm\infty$.

The existence of the *out* and *in vacuum states* $\omega_{\mathrm{out/in}}$ for a Klein-Gordon operator P on (M, g), i.e., of states looking like the Fock vacua for the static Klein-Gordon operators $P_{\mathrm{out/in}}$ on $(M, g_{\mathrm{out/in}})$ at large positive or negative times, is often taken for granted in the physics literature.

We will explain the result of **[GW3]**, which provides a proof of the existence of $\omega_{\mathrm{out/in}}$ and more importantly of their Hadamard property.

15.1. Klein-Gordon operators on asymptotically static spacetimes

Let us now introduce a class of spacetimes that are asymptotically static at future and past time infinity and corresponding Klein-Gordon operators We fix an $(n-1)$-dimensional manifold Σ and set $M = \mathbb{R}_t \times \Sigma_{\mathrm{y}}$, $y = (t, \mathrm{y})$. We equip M with the Lorentzian metric

$$g = -c^2(y)dt^2 + \big(dy^i + b^i(y)dt\big)h_{ij}(y)\big(dy^j + b^j(y)dt\big), \tag{15.1}$$

where $c \in C^\infty(M)$, $h(t, \mathrm{y})dy^2$, resp. $b(t, \mathrm{y})$ is a smooth t-dependent Riemannian metric, resp. vector field on Σ.

If there exist a reference Riemannian metric $k(\mathrm{y})dy^2$ on Σ and constants $c_0, c_1 > 0$ such that

$$h(t, \mathrm{y}) \leq c_1 k(\mathrm{y}), \quad b(t, \mathrm{y})\cdot h(t, \mathrm{y})b(t, \mathrm{y}) \leq c_1, \quad c_0 \leq c(t, \mathrm{y}) \leq c_1, \quad (t, \mathrm{y}) \in M, \tag{15.2}$$

then it follows from **[CC**, Theorem 2.1] that $t : M \to \mathbb{R}$ is a Cauchy temporal function for (M, g), see Definition 5.4.5, hence in particular (M, g) is globally hyperbolic.

It is natural to use the framework of bounded geometry and to equip Σ with a reference Riemannian metric k such that (Σ, k) is of bounded geometry. The version of (15.2) is then

$$\text{(bg)} \quad \begin{cases} h \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^0_2(\Sigma, k)), \quad h^{-1} \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^2_0(\Sigma, k)), \\ b \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^1_0(\Sigma, k)) \quad c, c^{-1} \in C^\infty_{\mathrm{b}}(\mathbb{R}; BT^0_0(\Sigma, k)). \end{cases} \tag{15.3}$$

A concrete example of (Σ, k) is $\mathbb{R}^d$ equipped with the uniform metric.

15.1.1. Asymptotically static spacetimes. Let us consider a Klein-Gordon operator

$$P = -(\nabla^\mu - \mathrm{i}qA^\mu(x))(\nabla_\mu - \mathrm{i}qA_\mu(x)) + V(x)$$

on (M,g). We now impose conditions on h,b,c,A,V which mean that (M,g) is *asymptotically static* at $t=\pm\infty$. Let us first introduce a convenient notation.

DEFINITION 15.1.1. *Let $\mathcal{F}$ be a Fréchet space whose topology is defined by the semi-norms $\|\cdot\|_n$, $n\in\mathbb{N}$. For $I\subset\mathbb{R}$ an interval, we denote by $S^\delta(I;\mathcal{F})$, $\delta\in\mathbb{R}$, the space of functions $I\ni t\mapsto X(t)\in\mathcal{F}$ such that*

$$\sup_{t\in I}\langle t\rangle^{-\delta+m}\|\partial_t^m X(t)\|_n<\infty,\ \ \forall\, m,n\in\mathbb{N}.$$

We introduce two static metrics

$$g_{\rm out/in}=-c^2_{\rm out/in}({\rm y})dt^2+h_{\rm out/in}({\rm y})d{\rm y}^2$$

and time-independent potentials $V_{\rm out/in}$ and assume the following conditions

$$\text{(as)}\quad\begin{cases} h(y)-h_{\rm out/in}({\rm y})\in S^{-\mu}(\mathbb{R}^\pm;BT^0_2(\Sigma,k)),\\ b(y)\in S^{-\mu'}(\mathbb{R};BT^1_0(\Sigma,k)),\quad A(y)\in S^{-\mu'}(\mathbb{R};BT^0_1(\Sigma,k)),\\ c(y)-c_{\rm out/in}({\rm y})\in S^{-\mu}(\mathbb{R}^\pm;BT^0_0(\Sigma,k)),\\ V(y)-V_{\rm out/in}({\rm y})\in S^{-\mu}(\mathbb{R}^\pm;BT^0_0(\Sigma,k)),\end{cases}$$

for some $\mu>0$, $\mu'>1$. Here the space $S^\delta(\mathbb{R};BT^p_q(\Sigma,k))$, $\delta\in\mathbb{R}$ is defined as in Definition 15.1.1.

The above conditions are standard scattering type conditions, with μ,μ' measuring the rate of convergence of h,b, etc. to their limits at $t=\pm\infty$. The condition $\mu'>1$ is traditionally called a *short-range* condition in the scattering theory for Schrödinger equations, while $\mu>0$ corresponds to the weaker *long-range* condition.

15.2. The *in* and *out* vacuum states

15.2.1. The asymptotic Klein-Gordon operators. It follows from condition (as) that when $t\to\pm\infty$, P is asymptotic to the Klein-Gordon operator

$$P_{\rm out/in}=-\Box_{g_{\rm out/in}}+V_{\rm out/in},$$

associated to the static metric $g_{\rm out/in}$. We can introduce the ultra-static metric

$$\tilde g_{\rm out/in}=c^{-2}_{\rm out/in}g_{\rm out/in}=-dt^2+\tilde h_{\rm out/in}({\rm y})d{\rm y}$$

and obtain from Section 6.3 that

$$P_{\rm out/in}=c^{-n/2-1}_{\rm out/in}\tilde P_{\rm out/in}c^{n/2-1}_{\rm out/in},$$

where

$$\tilde P_{\rm out/in}=-\Box_{\tilde g_{\rm out/in}}+\frac{n-2}{4(n-1)}{\rm Scal}_{\tilde g_{\rm out/in}}+c^{-2}_{\rm out/in}\tilde V_{\rm out/in},$$

and $\tilde V_{\rm out/in}=V_{\rm out/in}-\frac{n-2}{4(n-1)}{\rm Scal}_{g_{\rm out/in}}$. The ultra-static Klein-Gordon operator $\tilde P_{\rm out/in}$ equals $\partial_t^2+\tilde a_{\rm out/in}({\rm y},\partial_{\rm y})$, and to avoid technical complications coming from infrared problems we will assume that

$$\text{(pos)}\quad\frac{n-2}{4(n-1)}{\rm Scal}_{\tilde g_{\rm out/in}}+c^{-2}_{\rm out/in}\tilde V_{\rm out/in}\geq m^2,\ \ \text{for some } m>0,$$

which simply means that

$$\tilde a_{\rm out/in}\geq m^2>0\ \ \text{on } L^2(\Sigma,|\tilde h_{\rm out/in}|^{\frac12}({\rm y})d{\rm y}),$$

for $\tilde h_{\rm out/in}=c^{-2}_{\rm out/in}h_{\rm out/in}$.

It follows that $\tilde{P}_{\mathrm{out/in}}$ admits a *vacuum state* $\tilde{\omega}^{\mathrm{vac}}_{\mathrm{out/in}}$, see Subsection 4.10.2, whose Cauchy surface covariances are

$$\tilde{\lambda}^{\pm,\mathrm{vac}}_{\mathrm{out/in}} = \frac{1}{2}\begin{pmatrix} \tilde{\epsilon}_{\mathrm{out/in}} & \pm\mathbb{1} \\ \pm\mathbb{1} & \tilde{\epsilon}^{-1}_{\mathrm{out/in}} \end{pmatrix},\ \tilde{\epsilon}_{\mathrm{out/in}} = \tilde{a}^{\frac{1}{2}}_{\mathrm{out/in}}.$$

By Subsection 6.3.2, $P_{\mathrm{out/in}}$ admit the vacuum state $\omega^{\mathrm{vac}}_{\mathrm{out/in}}$, whose Cauchy surface covariances on $\Sigma_0 = \{0\}\times\Sigma$ are

$$\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}} = (U^*_{\mathrm{out/in}})^{-1}\circ\tilde{\lambda}^{\pm,\mathrm{vac}}_{\mathrm{out/in}}\circ U^{-1}_{\mathrm{out/in}},\quad U = \begin{pmatrix} c^{1-n/2}_{\mathrm{out/in}} & 0 \\ 0 & c^{-n/2}_{\mathrm{out/in}} \end{pmatrix}.$$

15.2.2. The *out* and *in* vacuum states. We have seen that $\Sigma_s = \{s\}\times\Sigma$ are Cauchy surfaces for (M,g). Denoting by $\varrho_s : \mathrm{Sol}_{\mathrm{sc}}(P) \to C^\infty_0(\Sigma_s;\mathbb{C}^2)$ the Cauchy data map on Σ_s, see (5.27) and by $U_s f$, $f\in C^\infty_0(\Sigma_s;\mathbb{C}^2)$, the solution of the Cauchy problem on Σ_s we set

$$\mathcal{U}(t,s) := \varrho_t U_s : C^\infty_0(\Sigma_s;\mathbb{C}^2) \longrightarrow C^\infty_0(\Sigma_t;\mathbb{C}^2).$$

If ω is a quasi-free state for P, with spacetime covariances $\Lambda^\pm$, we will denote by $\lambda^\pm_t$ its Cauchy surface covariances on Σ_t, called the *time t covariances* of the state ω.

From Propositions 5.5.4, 6.1.6 it easily follows that

$$\lambda^\pm_s = \mathcal{U}(t,s)^*\circ\lambda^\pm_t\circ\mathcal{U}(t,s),\quad s,t\in\mathbb{R}. \tag{15.4}$$

We would like to define quasi-free states $\omega_{\mathrm{out/in}}$ for P, called the *out/in vacua* which look like the 'free' vacua $\omega^{\mathrm{vac}}_{\mathrm{out/in}}$ when $t\to\pm\infty$. Taking (15.4) into account, we see that $\omega_{\mathrm{out/in}}$ should be defined by the time 0 covariances:

$$\lambda^\pm_{\mathrm{out/in}}(0) = \lim_{t\to\pm\infty}\mathcal{U}(t,0)^*\circ\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}}\circ\mathcal{U}(t,0), \tag{15.5}$$

where the limit above is taken as sesquilinear forms on $C^\infty_0(\Sigma_0;\mathbb{C}^2)$. Of course, the reference time $t=0$ is completely arbitrary.

The following theorem is the main result of **[GW3]**.

THEOREM 15.2.1. *Assume the conditions* (bg), (as) *and* (pos). *Then:*

(1) *the limits* (15.5) *when $t\to+\infty$, resp. $-\infty$, exist and are the time* 0 *covariances of a quasi-free state for P denoted by ω_{out}, resp. ω_{in}, called the* out *resp.* in vacuum state.
(2) *$\omega_{\mathrm{out/in}}$ are pure Hadamard states.*

15.2.3. Wave operators. The static vacua $\omega^{\mathrm{vac}}_{\mathrm{out/in}}$ are invariant under time translations: if $\mathcal{U}_{\mathrm{out/in}}(t,s)$ is the Cauchy evolution operator for $P_{\mathrm{out/in}}$, then $\mathcal{U}_{\mathrm{out/in}}(t,s) = \mathcal{U}_{\mathrm{out/in}}(t+T,s+T)$ and

$$\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}} = \mathcal{U}_{\mathrm{out/in}}(t,s)^*\circ\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}}\circ\mathcal{U}_{\mathrm{out/in}}(t,s).$$

Therefore we can rewrite (15.5) as

$$\lambda^\pm_{\mathrm{out/in}}(0) = \lim_{t\to\pm\infty}(\mathcal{U}_{\mathrm{out/in}}(0,t)\circ\mathcal{U}(t,0))^*\circ\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}}\circ(\mathcal{U}_{\mathrm{out/in}}(0,t)\circ\mathcal{U}(t,0)).$$

If the exponent μ in conditions (as) satisfies $\mu>1$, then one can prove that the strong limits

$$W_{\mathrm{out/in}} = \mathrm{s}\text{-}\lim_{t\to\pm\infty}\mathcal{U}_{\mathrm{out/in}}(0,t)\circ\mathcal{U}(t,0) \tag{15.6}$$

exist on some natural energy spaces. The operators $W_{\mathrm{out/in}}$ are called (*inverse*) *wave operators* and (15.5) takes the more familiar form

$$\lambda^\pm_{\mathrm{out/in}}(0) = W^*_{\mathrm{out/in}}\lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}}W_{\mathrm{out/in}},$$

which is often found in the physics literature. Note however that the existence of $W_{\mathrm{out/in}}$ requires $\mu > 1$, while the existence of $\omega_{\mathrm{out/in}}$ only requires $\mu > 0$.

15.3. Reduction to a model case

We now give some ideas of the proof of Theorem 15.2.1. The existence of $\omega_{\mathrm{out/in}}$, at least in the short-range case $\mu > 1$, is not very difficult, using the arguments outlined in Subsection 15.2.3.

The Hadamard property is more delicate. For example, the covariances $\mathcal{U}(t,0)^* \circ \lambda^{\pm,\mathrm{vac}}_{\mathrm{out/in}} \circ \mathcal{U}(t,0)$ in the right-hand side of (15.5) are *not* Hadamard for P for finite t. In fact, the free vacua $\omega^{\mathrm{vac}}_{\mathrm{out/in}}$ are Hadamard states for $P_{\mathrm{out/in}}$, but not for P. It is only after taking the limit $t \to \infty$ that one obtains a Hadamard state for P.

The proof of Theorem 15.2.1 is done by reduction to a model case, similar to the one considered in Section 11.2. Since we want to use the time coordinate t and not the Gaussian time, we use the orthogonal decomposition associated to t explained in Subsection 5.4.1.

15.3.1. Orthogonal decomposition. One can identify $\{0\} \times \Sigma$ with Σ and use the vector field

$$v = (\nabla t \cdot g \nabla t)^{-1} \nabla t = \partial_t + b^i(y)\partial_{\mathrm{y}^i}$$

as in Subsection 5.4.1 to construct an orthogonal decomposition of g by the diffeomorphism

$$\chi : \mathbb{R} \times \Sigma \ni (t, \mathrm{x}) \longmapsto (t, \mathrm{y}(t, 0, \mathrm{x})) \in \mathbb{R} \times \Sigma,$$

where $\mathrm{y}(t, s, \cdot) : \Sigma \to \Sigma$ is the flow of the time-dependent vector field $b^i(y)\partial_{\mathrm{y}^i}$ on Σ. The metric $\chi^* g$ takes the form

$$\chi^* g = \hat{c}^2(t, \mathrm{x})dt^2 + \hat{h}(t, \mathrm{x})d\mathrm{x}^2.$$

After a further conformal transformation, the operator

$$\tilde{P} := \hat{c}^{1-n/2} \chi^* P \hat{c}^{1+n/2}$$

take on the form, see [**GW3**, Subsection 5.2]

$$\tilde{P} = \partial_t^2 + r(t, \mathrm{x})\partial_t + a(t, \mathrm{x}, \partial_{\mathrm{x}}),$$

i.e. is a model Klein-Gordon operator of the type considered in Section 11.2.

15.3.2. Properties of the model operator. In the sequel the model operator $\tilde{P}$ will be denoted by P for simplicity.

Let us first introduce classes of time-dependent pseudodifferential operators on Σ that are analogs of the classes of time-dependent tensors $S^\delta(\mathbb{R}; BT^p_q(\Sigma, k))$ defined in Subsection 15.1.1. We set

$$\Psi^{m,\delta}_{\mathrm{td}}(I; \Sigma) := \mathrm{Op}(S^\delta(I; BS^m_{\mathrm{ph}}(\Sigma))) + S^\delta(I; \mathcal{W}^{-\infty}(\Sigma)),$$

where $BS^m_{\mathrm{ph}}(\Sigma)$ and $\mathcal{W}^{-\infty}(\Sigma)$ are defined in Definitions 10.4.1, 10.4.3, and we use Definition 15.1.1.

One can show that the conditions (bg), (as), (pos) imply the conditions

$$\text{(td)} \quad \begin{cases} a(t, \mathrm{x}, \partial_{\mathrm{x}}) = a_{\mathrm{out/in}}(\mathrm{x}, D_{\mathrm{x}}) + \Psi^{2,-\delta}_{\mathrm{td}}(\mathbb{R}^\pm; \Sigma), \ \delta > 0, \\ r(t) \in \Psi^{0,-1-\delta}_{\mathrm{td}}(\mathbb{R}; \Sigma), \\ a_{\mathrm{out/in}}(\mathrm{x}, \partial_{\mathrm{x}}) \in \Psi^2(\Sigma) \text{ elliptic}, \ a_{\mathrm{out/in}}(\mathrm{x}, D_{\mathrm{x}}) = a_{\mathrm{out/in}}(\mathrm{x}, D_{\mathrm{x}})^* \geq C_\infty > 0, \end{cases}$$

for $\delta = \min(\mu, \mu' - 1)$. The asymptotic Klein-Gordon operators are now

$$P_{\mathrm{out/in}} = \partial_t^2 + a_{\mathrm{out/in}}(\mathrm{x}, \partial_{\mathrm{x}}).$$

The decay conditions (td) lead to an improvement of the properties of the generator $b(t)$ constructed in Section 11.3. Indeed, setting $\epsilon(t) = a(t,x,\partial_x)^{\frac{1}{2}}$ and $\epsilon_{\rm out/in} = a^{\frac{1}{2}}_{\rm out/in}$ one can show that $b(t)$ in Proposition 11.3.1 can be chosen so that

$$\begin{aligned} &b(t) = \epsilon(t) + \Psi^{0,-1-\delta}_{\rm td}(\mathbb{R};^{\pm}\,\Sigma) = \epsilon_{\rm out/in} + \Psi^{1,-\delta}_{\rm td}(\mathbb{R}^{\pm};\Sigma),\\ &{\rm i}\partial_t b - b^2 + a + {\rm i}rb \in \Psi^{-\infty,-1-\delta}_{\rm td}(\mathbb{R};\Sigma). \end{aligned} \tag{15.7}$$

15.3.3. Almost diagonalization. In Chapter 11 the microlocal splitting deduced from a solution $b(t)$ was used to construct a pure Hadamard state. It is also possible, see [**GOW**, Section 6], to use it to diagonalize the evolution $\mathcal{U}(t,s)$ associated to P, modulo smoothing error terms. Let us set

$$T(t) := {\rm i}^{-1}\begin{pmatrix} \mathbb{1} & -\mathbb{1} \\ b^+ & -b^- \end{pmatrix}(b^+ - b^-)^{-\frac{1}{2}}(t),$$

where we recall that $b^+(t) = b(t)$, $b^-(t) = -b^*(t)$. Then one can check that

$$T^{-1}(t) = {\rm i}(b^+ - b^-)^{-\frac{1}{2}}\begin{pmatrix} -b^- & \mathbb{1} \\ -b^+ & \mathbb{1} \end{pmatrix}(t).$$

We now define

$$\mathcal{U}(t,s) =: T(t)\circ\mathcal{U}^{\rm ad}(t,s)\circ T(s)^{-1}, \quad t,s\in\mathbb{R} \tag{15.8}$$

which is (at least formally) a two-parameter group. Computing the infinitesimal generator of $\{\mathcal{U}^{\rm ad}(t,s)\}_{t,s\in\mathbb{R}}$ one obtains

$$H^{\rm ad}(t) = \begin{pmatrix} -b^- + r_b^- & 0 \\ 0 & -b^+ + r_b^+ \end{pmatrix}(t) + R_{-\infty}(t), \tag{15.9}$$

where $R_{-\infty} \in \Psi^{-\infty,-1-\delta}_{\rm td}(\mathbb{R};\Sigma)\otimes M(\mathbb{C}^2)$ and $r_b^{\pm} \in \Psi^{0,-1-\delta}_{\rm td}(\mathbb{R};\Sigma)$, i.e. $H^{\rm ad}(t)$ is diagonal, modulo the regularizing in space and decaying in time error term $R_{-\infty}(t)$. There is a similar well-known *exact* diagonalization of the Cauchy evolutions $\mathcal{U}_{\rm out/in}(t,s)$ for $P_{\rm out/in}$. If

$$T_{\rm out/in} = ({\rm i}\sqrt{2})^{-1}\begin{pmatrix} \epsilon_{\rm out/in}^{-\frac{1}{2}} & -\epsilon_{\rm out/in}^{-\frac{1}{2}} \\ \epsilon_{\rm out/in}^{\frac{1}{2}} & \epsilon_{\rm out/in}^{\frac{1}{2}} \end{pmatrix}, \quad \epsilon_{\rm out/in} = a^{\frac{1}{2}}_{\rm out/in},$$

then

$$\mathcal{U}_{\rm out/in}(t,s) = T_{\rm out/in}\circ\mathcal{U}^{\rm ad}_{\rm out/in}(t,s)\circ T^{-1}_{\rm out/in},$$

and the (time-independent) generator $H^{\rm ad}_{\rm out/in}$ of $\mathcal{U}^{\rm ad}_{\rm out/in}(t,s)$ equals

$$H^{\rm ad}_{\rm out/in} = \begin{pmatrix} \epsilon_{\rm out/in} & 0 \\ 0 & -\epsilon_{\rm out/in} \end{pmatrix}.$$

The vacua $\omega^{\rm vac}_{\rm out/in}$ are pure states associated to the projections

$$c^{\pm}_{\rm out/in} = T_{\rm out/in}\circ\pi^+\circ T^{-1}_{\rm out/in}, \quad \text{for } \pi^+ = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}, \pi^- = \mathbb{1} - \pi^+.$$

Rather straightforward arguments show that the existence of the limits in Theorem 15.2.1 follows from the existence of

$$\lim_{t\to\pm\infty} W_{\rm out/in}(t)\circ\pi^{\pm}\circ W_{\rm out/in}(t)^{-1}, \text{ for } W_{\rm out/in}(t) = \mathcal{U}^{\rm ad}(0,t)\mathcal{U}^{\rm ad}_{\rm out/in}(t,0), \tag{15.10}$$

for example in $B(L^2(\Sigma;\mathbb{C}^2))$. Using the properties of $H^{\rm ad}(t)$ one can actually prove that

$$\text{s}-\lim_{t\to\pm\infty} W_{\rm out/in}(t)\circ\pi^{\pm}\circ W_{\rm out/in}(t)^{-1} = \pi^{\pm} + \mathcal{W}^{-\infty}(\Sigma)\otimes M(\mathbb{C}^2). \tag{15.11}$$

This implies not only the existence of the out/in vacuum states, but also their Hadamard property. Indeed, if $c^\pm = T(0)\pi^\pm T(0)^{-1}$ then $\lambda^\pm(0) = \pm q \circ c^\pm$ are the Cauchy surface covariances on Σ_0 of the Hadamard state associated to the microlocal splitting obtained from b, see Section 11.4. From (15.11) we obtain that $\lambda^\pm_{\mathrm{out/in}}(0)$ differ from $\lambda^\pm(0)$ by a smoothing error, which proves that $\omega_{\mathrm{out/in}}$ are Hadamard states.

CHAPTER 16

Feynman propagator on asymptotically Minkowski spacetimes

We have seen in Section 7.4 that a Klein-Gordon operator P on a globally hyperbolic spacetime (M, g) possesses four *distinguished parametrices*, the *retarded/advanced* parametrices $\tilde{G}_{\mathrm{ret/adv}}$ and the *Feynman/anti-Feynman* parametrices $\tilde{G}_{\mathrm{F}/\overline{\mathrm{F}}}$, unique modulo smooth kernels and uniquely characterized by the wavefront set of their distributional kernels.

One can ask if there exist true *inverses* of P, corresponding to the above parametrices and canonically associated to the spacetime (M, g).

By Lemma 7.4.3, there exists true retarded/advanced inverses of P, namely $G_{\mathrm{ret/adv}}$, see Theorem 5.5.1, which are uniquely determined by the causal structure of (M, g).

The situation is more complicated for the Feynman/anti-Feynman inverses. Of course, given a Hadamard state ω for P, the Feynman inverse associated to ω, see (8.14), has the correct wavefront set, but it depends on the choice of the Hadamard state ω, and hence is not canonical.

There are some situations where such a canonical Feynman inverse exists. If (M, g) is stationary with Killing vector field X and P is invariant under X, one can, under the conditions in Chapter 9, construct the *vacuum state* ω_{vac} associated to X and the corresponding Feynman inverse G_{F} is a canonical choice of a Feynman inverse, respecting the symmetries of (M, g).

In the particular case of the Minkowski spacetime $\mathbb{R}^{1,d}$ and $P = \partial_t^2 - \Delta_x + m^2$, the Feynman inverse obtained from the vacuum state is equal to the Fourier multiplier by the distribution

$$\frac{-1}{\tau^2 - (k^2 + m^2) + \mathrm{i}0}.$$

In this chapter we will describe the results of **[GW4, GW6]**, devoted to this question on spacetimes which are *asymptotically Minkowski*, and hence have in general no global symmetries, only asymptotic ones.

It turns out that it is possible in this case to define a *canonical Feynman inverse* G_{F}, which is the inverse of P between some appropriate Sobolev type spaces.

More concretely, one introduces spaces $\mathcal{Y}^m$, $\mathcal{X}^m_{\mathrm{F}}$ for $m \in \mathbb{R}$, see Section 16.3, where $\mathcal{Y}^m$ is a space of functions decaying fast enough when $t \to \pm\infty$, while the functions in $\mathcal{X}^m_{\mathrm{F}}$ satisfy asymptotic conditions at $t = \pm\infty$ which are analogs of the wavefront set condition which characterizes Feynman parametrices.

One can show that $P : \mathcal{X}^m_F \to \mathcal{Y}^m$ is invertible, and that its inverse G_{F} is a Feynman parametrix in the sense of Subsection 7.4.2.

Vasy **[Va]** considered the same problem by working directly on the scalar operator P using microlocal methods. He constructed the Feynman inverse G_{F} between microlocal Sobolev spaces, as the boundary value $(P - \mathrm{i}0)^{-1}$ of the resolvent of P.

16.1. Klein-Gordon operators on asymptotically Minkowski spacetimes

In this subsection we recall the framework considered in **[GW4]**.

16.1.1. Asymptotically Minkowski spacetimes. We consider $M = \mathbb{R}^{1+d}$ equipped with a Lorentzian metric g such that

(aM(i)) $g_{\mu\nu}(x) - \eta_{\mu\nu} \in S^{-\delta}_{\rm std}(\mathbb{R}^{1+d}),\ \delta > 1,$

(aM(ii)) $(\mathbb{R}^{1+d}, g)$ is globally hyperbolic,

(aM(iii)) $(\mathbb{R}^{1+d}, g)$ has a temporal function $\tilde{t}$ with $\tilde{t} - t \in S^{1-\epsilon}_{\rm std}(\mathbb{R}^{1+d})$ for $\epsilon > 0$,

where $\eta_{\mu\nu}$ is the Minkowski metric and $S^{\delta}_{\rm std}(\mathbb{R}^{1+d})$ denotes the class of smooth functions f such that, for $\langle x\rangle = (1+|x|)^{\frac{1}{2}}$,

$$\partial_x^\alpha f \in O(\langle x\rangle^{\delta-|\alpha|}), \quad \alpha \in \mathbb{N}^{1+d}.$$

Recall that $\tilde{t}$ is called a *temporal function* if $\nabla\tilde{t}$ is a time-like vector field, and is called a *Cauchy temporal function* if in addition its level sets are Cauchy surfaces for (M, g).

It is shown in **[GW4]** that if (aM(i)) holds, then (aM(ii)) is equivalent to the familiar *non trapping condition* for null geodesics of g, and if (aM(i), (ii), (iii)) hold, then there exists a Cauchy temporal function $\tilde{t}$ such that $\tilde{t} - t \in C^\infty_0(M)$.

Replacing t by $t - c$, $\tilde{t}$ by $\tilde{t} - c$ for $c \gg 1$ we can also assume that $\Sigma := \{t = 0\} = \{\tilde{t} = 0\}$ is a Cauchy surface for (M, g), which can be canonically identified with $\mathbb{R}^d$. In the sequel we will fix such a temporal function $\tilde{t}$.

16.1.2. Klein-Gordon operator. We fix a real function $V \in C^\infty(M; \mathbb{R})$ such that

$$\text{(aM(iv))}\ \ V(x) - m^2 \in S^{-\delta}_{\rm std}(\mathbb{R}^{1+d}), \quad \text{for some } m > 0,\ \delta > 1,$$

and consider the Klein-Gordon operator

$$P = -\Box_g + V.$$

16.2. The Feynman inverse of P

We now introduce the Hilbert spaces $\mathcal{X}^m_{\rm F}$, $\mathcal{Y}^m$ between which P will be invertible. The spaces $\mathcal{Y}^m$ are standard spaces of right-hand sides for the Klein-Gordon equations, their essential property being that their elements are L^1 in t, with values in some Sobolev spaces of order m. The spaces $\mathcal{X}^m_{\rm F}$ incorporate the *Feynman boundary conditions*, which are imposed at $t = \pm\infty$.

16.2.1. Hilbert spaces. Using the Cauchy temporal function $\tilde{t}$ we can identify M with $\mathbb{R}\times\Sigma$ using the flow ϕ_t of the vector field $v = \frac{g^{-1}d\tilde{t}}{d\tilde{t}\cdot g^{-1}d\tilde{t}}$, and obtain the diffeomorphism

$$\chi : \mathbb{R}\times\Sigma \ni (t, \mathrm{x}) \longmapsto \phi_t(\mathrm{x}) \in M, \tag{16.1}$$

such that

$$\chi^* g = -c^2(t, \mathrm{x})dt^2 + h(t, \mathrm{x})d\mathrm{x}^2.$$

For $m \in \mathbb{R}$ we denote by $H^m(\mathbb{R}^d)$ the usual Sobolev spaces on $\mathbb{R}^d$. We set, for $\frac{1}{2} < \gamma < \frac{1}{2} + \delta$

$$\mathcal{Y}^m := \{u \in \mathcal{D}'(M) : \chi^* u \in \langle t\rangle^{-\gamma} L^2(\mathbb{R}; H^m(\mathbb{R}^d))\},$$

with norm $\|v\|_{\mathcal{Y}^m} = \|\chi^* u\|_{L^2(\mathbb{R}; H^m(\mathbb{R}^d))}$. The exponent γ is chosen such that $\langle t\rangle^{-\gamma} L^2(\mathbb{R}) \subset L^1(\mathbb{R})$. Similarly we set

$$\mathcal{X}^m := \{u \in \mathcal{D}'(M) : \chi^* u \in C^0(\mathbb{R}; H^{m+1}(\mathbb{R}^d)) \cap C^1(\mathbb{R}; H^m(\mathbb{R}^d)),\ Pu \in \mathcal{Y}^m\}.$$

We equip $\mathcal{X}^m$ with the norm

$$\|u\|_{\mathcal{X}^m} = \|\varrho_0 u\|_{\mathcal{E}^m} + \|Pu\|_{\mathcal{Y}^m},$$

where $\varrho_s u = \begin{pmatrix} u\restriction_{\Sigma_s} \\ \mathrm{i}^{-1}\partial_n u\restriction_{\Sigma_s} \end{pmatrix}$ is the Cauchy data map on $\Sigma_s := \tilde{t}^{-1}(\{s\})$ and $\mathcal{E}^m := H^{m+1}(\mathbb{R}^d)\oplus H^m(\mathbb{R}^d)$ is the energy space of order m. From the well-posedness of the inhomogeneous Cauchy problem for P one easily deduces that $\mathcal{X}^m$ is a Hilbert space.

16.2.2. Feynman boundary conditions. Let us set

$$c^{\pm}_{\text{free}} = \frac{1}{2}\begin{pmatrix} \mathbb{1} & \pm\sqrt{-\Delta_{\mathrm{x}} + m^2} \\ \pm\sqrt{-\Delta_{\mathrm{x}} + m^2} & \mathbb{1} \end{pmatrix}.$$

Of course, $\lambda^{\pm}_{\text{free}} = \pm q \circ c^{\pm}_{\text{free}}$ for $q = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ are the Cauchy surface covariances on Σ of the free vacuum state ω_{free} associated to P_{free}. We set then

$$\mathcal{X}^m_{\mathrm{F}} := \{u \in \mathcal{X}^m : \lim_{t\to\mp\infty} c^{\pm}_{\text{free}}\varrho_t u = 0 \text{ in } \mathcal{E}^m\}.$$

It is easy to see that $\mathcal{X}^m_{\mathrm{F}}$ is a closed subspace of $\mathcal{X}^m$.

The following theorem is proved in **[GW6]**.

THEOREM 16.2.1. *Assume* (aM). *Then $P : \mathcal{X}^m_{\mathrm{F}} \to \mathcal{Y}^m$ is boundedly invertible for all $m \in \mathbb{R}$. Its inverse G_{F} is called the* Feynman inverse *of P. It satisfies*

$$\mathrm{WF}(G_{\mathrm{F}})' = \Delta \cup \mathcal{C}_{\mathrm{F}}.$$

We recall that $\mathcal{C}_{\mathrm{F}}$ was defined in Section 7.4. In particular G_{F} is a Feynman parametrix for P.

16.3. Proof of Theorem 16.2.1

We now give some ideas of the proof of Theorem 16.2.1. As in Section 15.3, the first step consists in the reduction to a model Klein-Gordon equation, by using successively the diffeomorphism χ in Subsection 16.2.1 and the conformal transformation $\chi^* g \to c^{-2}(t,\mathrm{x})\chi^* g$. After this reduction, we work on $\mathbb{R}^{1+d}$ with elements $x = (t,\mathrm{x})$ equipped with the Lorentzian metric

$$g = -dt^2 + h_{ij}(t,\mathrm{x})d\mathrm{x}^i d\mathrm{x}^j,$$

where $t \mapsto h_t = h_{ij}(t,\mathrm{x})d\mathrm{x}^i d\mathrm{x}^j$ is a smooth family of Riemannian metrics on $\mathbb{R}^d$. The Klein-Gordon operator $P = -\Box_g + V$ takes the form

$$P = \partial_t^2 + r(t,\mathrm{x})\partial_t + a(t,\mathrm{x},\partial_{\mathrm{x}}), \tag{16.2}$$

where

$$a(t) = a(t,\mathrm{x},\partial_{\mathrm{x}}) = -|h|^{-\frac{1}{2}}\partial_i h^{ij}|h|^{\frac{1}{2}}\partial_j + V(t,\mathrm{x}),$$
$$r(t) = r(t,\mathrm{x}) = |h|^{-\frac{1}{2}}\partial_t(|h|^{\frac{1}{2}})(t,\mathrm{x}).$$

The operator $a(t)$ is formally selfadjoint for the time-dependent scalar product

$$(u|v)_t = \int_\Sigma \overline{u}v|h_t|^{\frac{1}{2}}d\mathrm{x},$$

and P is formally selfadjoint for the scalar product

$$(u|v) = \int_{\mathbb{R}\times\Sigma} \overline{u}v|h_t|^{\frac{1}{2}}d\mathrm{x}dt.$$

Conditions (aM) on the original metric g and potential V imply similar asymptotic conditions on $a(t,\mathrm{x},\partial_\mathrm{x})$ and $r(t,\mathrm{x})$ when $t\to\pm\infty$. More precisely, one has

$$\text{(Hstd)}\quad\begin{cases} a(t,\mathrm{x},\partial_\mathrm{x}) = a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x}) + \Psi^{2,-\delta}_{\mathrm{std}}(\mathbb{R}^\pm;\mathbb{R}^d),\\ r(t)\in\Psi^{0,-1-\delta}_{\mathrm{std}}(\mathbb{R};\mathbb{R}^d),\\ a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x})\in\Psi^{2,0}_{\mathrm{sc}}(\mathbb{R}^d) \text{ is elliptic},\\ a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x}) = a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x})^* \geq C_\infty > 0, \end{cases}$$

where $\Psi^{m,\delta}_{\mathrm{std}}(\mathbb{R}^\pm;\mathbb{R}^d)$ is the class of time-dependent pseudodifferential operators on $\mathbb{R}^d$ associated to symbols $m(t,\mathrm{x},k)$ such that

$$\partial_t^\gamma\partial_\mathrm{x}^\alpha\partial_k^\beta m(t,\mathrm{x},k)\in O((\langle t\rangle+\langle \mathrm{x}\rangle)^{\delta-\gamma-|\alpha|}\langle k\rangle^{m-|\beta|}),\quad \gamma\in\mathbb{N},\ \alpha,\beta\in\mathbb{N}^d,\ t\in\mathbb{R}^\pm.$$

Similarly, $\Psi^{m,\delta}_{\mathrm{sc}}(\mathbb{R}^d)$ is the class of pseudodifferential operators on $\mathbb{R}^d$ associated to symbols $m(\mathrm{x},k)$ such that

$$\partial_\mathrm{x}^\alpha\partial_k^\beta m(\mathrm{x},k)\in O(\langle \mathrm{x}\rangle^{\delta|\alpha|}\langle k\rangle^{m-|\beta|}),\quad \alpha,\beta\in\mathbb{N}^d.$$

We refer the reader to [**GW4**, Subsection 2.3] for more details.

The Hilbert spaces $\mathcal{Y}^m$ and $\mathcal{X}^m$ become

$$\mathcal{Y}^m = \langle t\rangle^{-\gamma}L^2(\mathbb{R};H^m(\mathbb{R}^d)),$$
$$\mathcal{X}^m = \{u\in C^0(\mathbb{R};H^{m+1}(\mathbb{R}^d))\cap C^1(\mathbb{R};H^m(\mathbb{R}^d)) : Pu\in\mathcal{Y}^m\},$$

equipped with the norm

$$\|u\|^2_{\mathcal{X}^m} = \|\varrho_0 u\|^2_{\mathcal{E}^m} + \|Pu\|^2_{\mathcal{Y}^m},$$

where $\varrho_t u = \begin{pmatrix} u(t)\\ \mathrm{i}^{-1}\partial_t u(t)\end{pmatrix}$ and the energy space $\mathcal{E}^m$ is defined in Subsection 16.2.1.

The subspaces $\mathcal{X}^m_{\mathrm{F}}$ become

$$\mathcal{X}^m_{\mathrm{F}} := \{u\in\mathcal{X}^m : \lim_{t\to-\infty} c^-_{\mathrm{out}}\varrho_t u = \lim_{t\to+\infty} c^+_{\mathrm{in}}\varrho_t u = 0 \text{ in } \mathcal{E}^m\}$$

where

$$c^\pm_{\mathrm{out/in}} = \frac{1}{2}\begin{pmatrix} 1 & \pm a^{\frac12}_{\mathrm{out/in}}\\ \pm a^{\frac12}_{\mathrm{out/in}} & 1\end{pmatrix}$$

are the projections for the out/in vacuum state $\omega_{\mathrm{out/in}}$ associated to the Klein-Gordon operator $\partial_t^2 + a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x})$.

16.3.1. A further reduction. It is convenient to perform a further reduction to the case $r=0$. Namely, setting $R = |h_0|^{\frac14}|h_t|^{-\frac14}$, we see that

$$L^2(\Sigma,|h_0|^{\frac12}d\mathrm{x})\ni\tilde u\longmapsto R\tilde u\in L^2(\Sigma,|h_t|^{\frac12}d\mathrm{x})$$

is unitary and that

$$R^{-1}PR =: \tilde P = \partial_t^2 + \tilde a(t,\mathrm{x},\partial_\mathrm{x}),$$

where

$$\tilde a(t) = rR^{-1}\partial_t R + R^{-1}(\partial_t^2 R) + R^{-1}a(t)R$$

is formally selfadjoint for $(\cdot|\cdot)_0$. Clearly, $\tilde a(t,\mathrm{x},\partial_\mathrm{x})$ satisfies also (Hstd), with the same asymptotic $a_{\mathrm{out/in}}(\mathrm{x},\partial_\mathrm{x})$. It is also immediate that the Hilbert spaces $\mathcal{Y}^m$, $\mathcal{X}^m$ and $\mathcal{X}^m_{\mathrm{F}}$ introduced in Section 2.2 are invariant under the map $u\mapsto Ru$ and hence we can assume that $r(t,\mathrm{x})=0$.

16.3.2. Almost diagonalization. One can then perform the same almost diagonalization as in Subsection 15.3.3. The stronger spacetime decay in conditions (Hstd) give stronger decay conditions on the off diagonal terms. More precisely, if $H(t) = \begin{pmatrix} 0 & \mathbb{1} \\ a(t) & 0 \end{pmatrix}$ is the generator of the Cauchy evolution for P and $T(t)$ is as in Subsection 15.3.3 we have

$$T^{-1}(D_t - H(t))T = D_t - H^{\rm ad}(t) =: P^{\rm ad},$$

where $H^{\rm ad}(t)$ is almost diagonal, i.e.

$$H^{\rm ad}(t) = H^{\rm d}(t) + V^{\rm ad}_{-\infty}(t),$$

$$H^{\rm d}(t) = \begin{pmatrix} \epsilon^+(t) & 0 \\ 0 & \epsilon^-(t) \end{pmatrix}, \tag{16.3}$$

where $\epsilon^{\pm}(t)$ belong to $\Psi^{1,0}(\mathbb{R};\mathbb{R}^d)$, with principal symbols equal to $\pm(kh^{-1}(t,\mathrm{x})k)^{\frac{1}{2}}$, and $V^{\rm ad}_{-\infty}(t)$ is an off-diagonal matrix of time-dependent operators on $\mathbb{R}^d$ such that

$$(\langle \mathrm{x}\rangle + \langle t\rangle)^m V^{\rm ad}_{-\infty}(t)(\langle \mathrm{x}\rangle + \langle t\rangle)^{-m+\delta} : H^{-p}(\mathbb{R}^d) \longrightarrow H^p(\mathbb{R}^d) \tag{16.4}$$

is uniformly bounded in t for all $m, p \in \mathbb{R}$. Compared with the situation in Section 15.3, we obtain extra decay in x and hence compactness properties of $V^{\rm ad}_{-\infty}$.

We denote by $\mathcal{U}(t,s)$, resp. $\mathcal{U}^{\rm ad}(t,s)$, for $t,s \in \mathbb{R}$, the Cauchy evolution generated by $H(t)$, resp. $H^{\rm ad}(t)$. Recall from (15.8) that

$$\mathcal{U}(t,s) = T(t) \circ \mathcal{U}^{\rm ad}(t,s) \circ T(s)^{-1}. \tag{16.5}$$

Moreover, $\mathcal{U}(t,s)^{(\rm ad)}$ are unitary with respect to the Hermitian scalar product

$$\overline{f}\cdot q^{(\rm ad)} g = (f|q^{(\rm ad)}g)_{\mathcal{H}^0},\ q = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix},\ q^{\rm ad} := \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \tag{16.6}$$

where $\mathcal{H}^0 = L^2(\mathbb{R}^d, |h_0|^{\frac{1}{2}}d\mathrm{x};\mathbb{C}^2)$, which implies the identity

$$H^{\rm ad}(t)^* q^{\rm ad} = q^{\rm ad} H^{\rm ad}(t), \tag{16.7}$$

where the adjoint is computed with respect to the scalar product of $\mathcal{H}^0$.

The spaces corresponding to $\mathcal{Y}^m$, $\mathcal{X}^m_{\rm F}$ with the scalar operator P replaced by the matrix operator $D_t - H^{\rm ad}(t)$ are the following:

$$\mathcal{Y}^{{\rm ad},m} = \langle t\rangle^{-\gamma} L^2(\mathbb{R}, \mathcal{H}^m),$$

$$\mathcal{X}^{{\rm ad},m} = \{u^{\rm ad} \in C^0(\mathbb{R};\mathcal{H}^{m+1}) \cap C^1(\mathbb{R};\mathcal{H}^m) : P^{\rm ad}u^{\rm ad} \in \mathcal{Y}^{{\rm ad},m}\},$$

equipped with the norm

$$\|u^{\rm ad}\|^2_{\mathcal{X}^{{\rm ad},m}} = \|\varrho_0 u^{\rm ad}\|^2_{\mathcal{H}^m} + \|P^{\rm ad}u\|^2_{\mathcal{Y}^{{\rm ad},m}},$$

where $\mathcal{H}^m = H^m(\mathbb{R}^d) \oplus H^m(\mathbb{R}^d)$ and $\varrho^{\rm ad}_t u^{\rm ad} = u^{\rm ad}(t)$. The subspace $\mathcal{X}^{{\rm ad},m}_{\rm F}$ is defined as

$$\mathcal{X}^{{\rm ad},m}_{\rm F} := \{u^{\rm ad} \in \mathcal{X}^{{\rm ad},m} : \lim_{t\to-\infty} \pi^+ \varrho^{\rm ad}_t u^{\rm ad} = \lim_{t\to+\infty} \pi^- \varrho^{\rm ad}_t u^{\rm ad} = 0 \text{ in } \mathcal{H}^m\},$$

where

$$\pi^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},\ \pi^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Note that $\pi^{\pm}$ are the spectral projections on $\mathbb{R}^{\pm}$ for the Hamiltonian

$$H^{\rm ad}_{\rm out/in} = \begin{pmatrix} a^{\frac{1}{2}}_{\rm out/in} & 0 \\ 0 & -a^{\frac{1}{2}}_{\rm out/in} \end{pmatrix}$$

and we will denote by $\mathcal{U}^{\rm ad}_{\rm out/in}(t,s)$ the evolution generated by $H^{\rm ad}_{\rm out/in}$.

PROPOSITION 16.3.1. *Assume* (aM). *Then the operator* $P^{\rm ad} : \mathcal{X}_{\rm F}^{{\rm ad},m} \to \mathcal{Y}^m$ *is Fredholm of index* 0.

Proof. Set $P^{\rm d} = D_t - H^{\rm d}(t)$. Then $P^{\rm d} : \mathcal{X}_{\rm F}^{{\rm ad},m} \to \mathcal{Y}^{{\rm ad},m}$ is boundedly invertible, with inverse $G_{\rm F}^{\rm d}$ given by

$$\begin{aligned} G_{\rm F}^{\rm d} v^{\rm ad}(t) \quad &:= {\rm i}\int_{-\infty}^{t} \mathcal{U}^{\rm d}(t,0)\pi^{+}\mathcal{U}^{\rm d}(0,s)v^{\rm ad}(s)ds \\ &\quad - {\rm i}\int_{t}^{+\infty} \mathcal{U}^{\rm d}(t,0)\pi^{-}\mathcal{U}^{\rm d}(0,s)v^{\rm ad}(s)ds. \end{aligned}$$

It is easy to show, see [**GW4**, Lemma 3.7], that $V_{-\infty}^{\rm ad}$ is compact from $\mathcal{X}^{{\rm ad},m}$ to $\mathcal{Y}^m$, hence also from $\mathcal{X}_{\rm F}^{{\rm ad},m}$ to $\mathcal{Y}^m$ since $\mathcal{X}_{\rm F}^{{\rm ad},m}$ is closed in $\mathcal{X}^{{\rm ad},m}$. □

Now let us prove that $P^{\rm ad} : \mathcal{X}_{\rm F}^{{\rm ad},m} \to \mathcal{Y}^m$ is injective, and hence boundedly invertible by Proposition 16.3.1. The proof of Lemma 16.3.2 below is inspired by the work of Vasy [**Va**, Proposition 7], which in turn relies on arguments of Isozaki [**I**] from N-body scattering theory.

LEMMA 16.3.2. *One has:*

$$\operatorname{Ker} P^{\rm ad}|_{\mathcal{X}_{\rm F}^{{\rm ad},m}} = \{0\} \text{ for all } m \in \mathbb{R}.$$

Proof. We first note that if $u^{\rm ad} \in \operatorname{Ker} P^{\rm ad}|_{\mathcal{X}_{\rm F}^{{\rm ad},m}}$, we have $u^{\rm ad} = -G_{\rm F}^{\rm d} V_{-\infty}^{\rm ad} u^{\rm ad}$, from which we deduce that $u^{\rm ad} \in \mathcal{X}_{\rm F}^{{\rm ad},m'}$ for any m', using that $V_{-\infty}^{\rm ad}$ is smoothing in x. Therefore, it suffices to prove the lemma for $m \geq 1$.

Let us set $\chi_\epsilon(t) = \int_{|t|}^{+\infty} \mathbb{1}_{[1,2]}(\epsilon s) s^{-r} ds$ for some $0 < r < 1$. Note that $\operatorname{supp}\chi_\epsilon \subset \{|t| \leq 2\epsilon^{-1}\}$. Let us still denote by χ_ϵ the operator $\chi_\epsilon \otimes \mathbb{1}_{\mathbb{C}^2}$. Recalling that $q^{\rm ad}$ is defined in (16.6), we compute for $u \in \mathcal{X}_{\rm F}^{{\rm ad},m}$:

$$\begin{aligned} &\int_{\mathbb{R}} \big(P^{\rm ad}u^{\rm ad}(t)|q^{\rm ad}\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0} - \big(\chi_\epsilon(t)u^{\rm ad}(t)|q^{\rm ad}P^{\rm ad}u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt \\ = &\int_{\mathbb{R}} \big(D_t u^{\rm ad}(t)|q^{\rm ad}\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0} - \big(u^{\rm ad}(t)|q^{\rm ad}\chi_\epsilon(t)D_t u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt \\ &+\int_{\mathbb{R}} \big(u^{\rm ad}(t)|q^{\rm ad}[H^{\rm ad}(t),\chi_\epsilon(t)]u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt, \end{aligned}$$

using that $H^{{\rm ad}*}(t)q^{\rm ad} = q^{\rm ad}H^{\rm ad}(t)$, $\chi_\epsilon(t)^* q^{\rm ad} = q^{\rm ad}\chi_\epsilon(t)$ and $u^{\rm ad}(t) \in \operatorname{Dom} H^{\rm ad}(t)$ since $m \geq 1$. We have $[H^{\rm ad}(t), \chi_\epsilon(t)] = 0$, and since χ_ϵ is compactly supported in t we can integrate by parts in t in the second line and obtain

(16.8)
$$\begin{aligned} &\int_{\mathbb{R}} \big(P^{\rm ad}u^{\rm ad}(t)|q^{\rm ad}\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt - \int_{\mathbb{R}} \big(\chi_\epsilon(t)u^{\rm ad}(t)|q^{\rm ad}P^{\rm ad}u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt \\ = &-{\rm i}\int_{\mathbb{R}} \big(u^{\rm ad}(t)|q^{\rm ad}\partial_t\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt. \end{aligned}$$

Note that we used here that the scalar product in $\mathcal{H}^0$ does not depend on t, which is the reason for the reduction to $r = 0$ in Subsection 16.3.1.

Since $P^{\rm ad}u^{\rm ad} = 0$, this yields

$$\int_{\mathbb{R}} \big(u^{\rm ad}(t)|q^{\rm ad}\partial_t\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt = 0. \tag{16.9}$$

We claim that:

$$\begin{aligned} &\text{(i)} \quad \|\pi^{\pm}u^{\rm ad}(t)\|^2_{\mathcal{H}^0} \in O(t^{1-\delta}), \text{ when } t \to \mp\infty, \\ &\text{(ii)} \quad \|\pi^{\pm}u^{\rm ad}(t)\|^2_{\mathcal{H}^0} = c^{\pm} + O(t^{1-\delta}), \text{ when } t \to \pm\infty, \end{aligned} \tag{16.10}$$

for $c^\pm = \lim_{t\to\pm}\|\pi^\pm u^{\rm ad}(t)\|^2_{\mathcal{H}^0}$. The proof of (16.10) is elementary: we have $H^{\rm ad}(t) - H^{\rm ad}_{\rm out/in} \in O(t^{-\delta})$ in $B(\mathcal{H}^0)$ when $t\to\pm\infty$, see e.g. [**GW1**, Subsection 2.5], which using that $\delta>1$ and the Cook argument yields

$$W^\dagger_{\rm out/in}u^{\rm ad} = \lim_{t\to\pm}\mathcal{U}^{\rm ad}_{\rm out/in}(0,t)u^{\rm ad}(t) \text{ exists in } \mathcal{H}^0,$$
$$\|W^\dagger_{\rm out/in}u^{\rm ad} - \mathcal{U}^{\rm ad}_{\rm out/in}(0,t)u^{\rm ad}(t)\|_{\mathcal{H}^0}\in O(t^{1-\delta}).$$

Since $\mathcal{U}^{\rm ad}_{\rm out/in}(0,t)$ is unitary on $\mathcal{H}^0$, this yields (16.10). We then compute

$$\begin{aligned}&\int_{\mathbb{R}}\big(u^{\rm ad}(t)|q^{\rm ad}\partial_t\chi_\epsilon(t)u^{\rm ad}(t)\big)_{\mathcal{H}^0}dt\\ =\ &\int_{\mathbb{R}}\partial_t\chi_\epsilon(t)\|\pi^+u^{\rm ad}(t)\|^2_{H^0}dt - \int_{\mathbb{R}}\partial_t\chi_\epsilon(t)\|\pi^-u^{\rm ad}(t)\|^2_{H^0}dt =: I^+ + I^-.\end{aligned}$$

Since $\partial_t\chi_\epsilon(t) = -{\rm sgn}(t)\mathbb{1}_{[\epsilon^{-1},2\epsilon^{-1}]}(|t|)|t|^{-r}$, we have, using (16.10):

$$0\le\int_{\mathbb{R}^\mp}|\partial_t\chi_\epsilon(t)|\|\pi^\pm u^{\rm ad}(t)\|^2_{H^0}dt \le C\int\mathbb{1}_{[\epsilon^{-1},2\epsilon^{-1}]}(|t|)|t|^{-r-\delta+1}dt\in O(\epsilon^{r+\delta-2}),$$

$$\begin{aligned}\int_{\mathbb{R}^\pm}\partial_t\chi_\epsilon(t)\|\pi^\pm u^{\rm ad}(t)\|^2_{H^0}dt &= \mp\int_{\mathbb{R}^\pm}\mathbb{1}_{[\epsilon^{-1},2\epsilon^{-1}]}(|t|)c^+|t|^{-r}dt + O(\epsilon^{r+\delta-2})\\ &= \mp Cc^\pm\epsilon^{r-1}+O(\epsilon^{r+\delta-1}).\end{aligned}$$

Using (16.9), this yields $C\epsilon^{r-1}(c^+ + c^-)\in O(\epsilon^{r+\delta-2})$, hence $c^+=c^-=0$, since $\delta>1$. Therefore by (16.10) we have $\lim_{t\to\pm\infty}\|u^{\rm ad}(t)\|_{\mathcal{H}^0}=0$. Since the Cauchy evolution $\mathcal{U}^{\rm ad}(t,s)$ is uniformly bounded in $B(\mathcal{H}^0)$ we have $u^{\rm ad}(0)=0$, hence $u=0$. □

The reduction explained at the beginning of Section 16.3 shows that Theorem 16.2.1 follows from

THEOREM 16.3.3. *$P:\mathcal{X}^m_{\rm F}\to\mathcal{Y}^m$ is boundedly invertible, with inverse*

$$G_{\rm F} = -\pi_0 T G^{\rm ad}_{\rm F}T^{-1}\pi_1^*.$$

Moreover, $G_{\rm F}$ is a Feynman inverse *of P, i.e.*

$$\mathrm{WF}(G_{\rm F})' = \Delta\cup\mathcal{C}_{\rm F}. \tag{16.11}$$

Proof. It is straightforward using the expression of T to check that

$$\pi_0 T\in B(\mathcal{X}^{{\rm ad},m+\frac12},\mathcal{X}^m),\ T^{-1}\pi_1^*\in B(\mathcal{Y}^m,\mathcal{Y}^{{\rm ad},m+\frac12}),$$

and so $G_{\rm F}:\mathcal{Y}^m\to\mathcal{X}^m$. Since $(D_t-H(t))TG^{\rm ad}_{\rm F}T^{-1} = TG^{\rm ad}_{\rm F}T^{-1}(D_t-H(t)) = \mathbb{1}$, we obtain that $PG_{\rm F}=G_{\rm F}P=\mathbb{1}$. We have also $\varrho\pi_0TG^{\rm ad}_{\rm F}T^{-1}\pi_1^* = TG^{\rm ad}_{\rm F}T^{-1}\pi_1^*v$. From [**GW4**, equ. (3.25)] we obtain that $\pi_0T:\mathcal{X}^{{\rm ad},m+\frac12}_{\rm F}\to\mathcal{X}^m_{\rm F}$, hence $\varrho_{\overline{\rm F}}G_{\rm F}=0$, i.e. $G_{\rm F}:\mathcal{Y}^m\to\mathcal{X}^m_{\rm F}$.

To prove the second statement, let $\tilde G_{\rm F} = -\pi_0TG^{\rm d}_{\rm F}T^{-1}\pi_1^*$. We have $G^{\rm d}_{\rm F}-G^{\rm ad}_{\rm F} =: R_{-\infty} = G^{\rm d}_{\rm F}V^{\rm ad}_{-\infty}G^{\rm ad}_F$ by the resolvent identity. It is shown in [**GW1**, Lemma 3.7] that $V^{\rm ad}_{-\infty}:\mathcal{X}^{{\rm ad},m}\to\mathcal{Y}^{m'}$ is bounded for all $m'>m$, hence $R_{-\infty}:\mathcal{Y}^{{\rm ad},m}\to\mathcal{X}^{{\rm ad},m'}$ for all $m'>m$, i.e. is smoothing in the x variables. We use then that $D_tR_{-\infty} = H^d(t)R_{-\infty}+V^{\rm ad}_{-\infty}G^{\rm ad}_F$, $R_{-\infty}D_t = R_{-\infty}H^{\rm ad}(t)+G^{\rm d}_{\rm F}V^{\rm ad}_{-\infty}$ to gain regularity in the t variable and obtain that $R_{-\infty}:\mathcal{E}'(\mathbb{R}^{1+d};\mathbb{C}^2)\to C^\infty(\mathbb{R}^{1+d};\mathbb{C}^2)$. Therefore, $G_{\rm F}-\tilde G_{\rm F}$ is a smoothing operator.

Let also $G_{\rm F,ref}$ be defined as $\tilde G_{\rm F}$ with $\mathcal{U}^{\rm d}(t,s)$ replaced by $\mathcal{U}^{\rm ad}(t,s)$. From (16.4) it follows that $\mathcal{U}^{\rm d}(\cdot,\cdot)-\mathcal{U}^{\rm ad}(\cdot,\cdot)$, and hence $G_{\rm F,ref}-\tilde G_{\rm F}$ have smooth kernels in $M\times M$.

Using (16.5), we see that $G_{\mathrm{F,ref}}$ is the Feynman inverse associated to a Hadamard state, see Theorems 11.4.1, 11.5.1. Therefore, $\mathrm{WF}(G_{\mathrm{F,ref}})' = \Delta \cup \mathcal{C}_{\mathrm{F}}$, which completes the proof of the theorem. □

CHAPTER 17

Dirac fields on curved spacetimes

In this chapter we will give a brief description of quantized Dirac fields on curved spacetimes. Usually Dirac equations on a Lorentzian manifold are introduced starting from *spin structures*, see [**Di2, Li2**] or [**LM**, Chaps. 1, 2]. Here we use the approach through *spinor bundles*, with which analysts may be more comfortable. We will follow the exposition by Trautman [**T**] and refer to [**FT**] for a comparison between the two approaches.

The quantization of Dirac fields on curved spacetimes is due to Dimock [**Di2**]. The definition of Hadamard states for quantized Dirac fields on globally hyperbolic spacetimes was given by Hollands [**Ho1**] and Sahlmann and Verch [**SV2**] and is completely analogous to the Klein-Gordon case. Another nice reference is [**S4**].

The *massless* Dirac equation can be written as a pair of uncoupled *Weyl equations* which were for some time supposed to describe *neutrinos* and *anti-neutrinos*. We describe the quantization of the Weyl equation, the corresponding definition of Hadamard states, and the relationship between Hadamard states for Weyl and for Dirac fields.

17.1. CAR $*$-algebras and quasi-free states

The fermionic version of Chapter 4, namely CAR $*$- algebras and quasi-free states on them, is quite parallel to the bosonic case. A detailed exposition can be found for example in [**DG**, Sections 12.5, 17.2]. The complex case, corresponding to *charged fermions*, is the most important in practice, although the real case corresponding to *neutral* or *Majorana fermions* is sometimes also considered. For simplicity we will only consider the complex case.

Definition 17.1.1. *Let $(\mathcal{Y}, \nu)$ be a pre-Hilbert space. The* CAR $*$-algebra *over $(\mathcal{X}, \nu)$, denoted by* $\mathrm{CAR}(\mathcal{Y}, \nu)$*, is the unital complex $*$-algebra generated by elements $\psi(y)$, $\psi^*(y)$, $y \in \mathcal{Y}$, with the relations*

$$
\begin{aligned}
&\psi(y_1 + \lambda y_2) = \psi(y_1) + \overline{\lambda}\psi(y_2),\\
&\psi^*(y_1 + \lambda y_2) = \psi(y_1) + \lambda\psi^*(y_2), \quad y_1, y_2 \in \mathcal{Y}, \lambda \in \mathbb{C},\\
&[\psi(y_1), \psi(y_2)]_+ = [\psi^*(y_1), \psi^*(y_2)]_+ = 0,\\
&[\psi(y_1), \psi^*(y_2)]_+ = \overline{y}_1 \cdot \nu y_2 \mathbb{1}, \quad y_1, y_2 \in \mathcal{Y},\\
&\psi(y)^* = \psi^*(y),
\end{aligned}
\tag{17.1}
$$

where $[A, B]_+ = AB + BA$ is the anti-commutator.

Quasi-free states on $\mathrm{CAR}(\mathcal{Y}, \nu)$ are defined in a way quite similar to the bosonic case.

Definition 17.1.2. *A state ω on* $\mathrm{CAR}(\mathcal{Y}, \nu)$ *is a* (*gauge invariant*) quasi-free state *if*

$$
\begin{aligned}
&\omega(\textstyle\prod_{i=1}^n \psi^*(y_i) \prod_{j=1}^m \psi(y'_j)) = 0, \quad \text{if } n \neq m,\\
&\omega(\textstyle\prod_{i=1}^n \psi^*(y_i) \prod_{j=1}^n \psi(y'_j)) = \sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) \prod_{i=1}^n \omega(\psi^*(y_i \psi(y_{\sigma(i)}))).
\end{aligned}
$$

A quasi-free state is again characterized by its covariances $\lambda^{\pm} \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$, defined by

$$\omega(\psi(y_1)\psi^*(y_2)) =: \overline{y}_1 \cdot \lambda^+ y_2, \quad \omega(\psi^*(y_2)\psi(y_1)) =: \overline{y}_1 \cdot \lambda^- y_2, \quad y_1, y_2 \in \mathcal{Y}.$$

One has the following analog of Proposition 4.7.6.

PROPOSITION 17.1.3. *Let $\lambda^{\pm} \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$. Then the following statements are equivalent:*

(1) *$\lambda^{\pm}$ are the covariances of a gauge invariant quasi-free state on* $\mathrm{CAR}(\mathcal{Y}, \nu)$*;*
(2) *$\lambda^{\pm} \geq 0$ and $\lambda^+ + \lambda^- = \nu$.*

Let us note an important difference with the bosonic case. Since $\nu > 0$, one can always consider the completion $(\mathcal{Y}^{\mathrm{cpl}}, \nu)$ of $(\mathcal{Y}, \nu)$ and uniquely extend any quasi-free state ω to $\mathrm{CAR}(\mathcal{Y}^{\mathrm{cpl}}, \nu)$. This is related to the fact that the $*$-algebra $\mathrm{CAR}(\mathcal{Y}, \nu)$ can be equipped with a unique C^*-norm, see e.g. [**DG**, Proposition 12.50]. Therefore, if necessary, one can assume that $(\mathcal{Y}, \nu)$ is a Hilbert space.

Let us conclude this subsection with the characterization of pure quasi-free states, see e.g. [**DG**, Theorem 17.31].

PROPOSITION 17.1.4. *A quasi-free state ω on* $\mathrm{CAR}(\mathcal{Y}, \nu)$ *is pure iff there exist projections $c^{\pm} \in L(\mathcal{Y})$ such that*

$$\lambda^{\pm} = \nu \circ c^{\pm}, \quad c^+ + c^- = \mathbb{1}.$$

Note that $c^{\pm}$ are bounded selfadjoint projections on $(\mathcal{Y}, \nu)$.

17.2. Clifford algebras

We now collect some standard facts about Clifford algebras. For simplicity, we will only discuss the case of Lorentzian signature. Let $\mathcal{X}$ be an n-dimensional real vector space and $\nu \in L_{\mathrm{h}}(\mathcal{X}, \mathcal{X}')$ be a symmetric non-degenerate bilinear form of signature $(1, d)$.

DEFINITION 17.2.1. *The* Clifford algebra $\mathrm{Cliff}(\mathcal{X}, \nu)$ *is the abstract* real *algebra generated by the elements $\gamma(x)$, $x \in \mathcal{X}$, and the relations*

$$\gamma(x_1 + \lambda x_2) = \gamma(x_1) + \lambda\gamma(x_2),$$
$$\gamma(x_1)\gamma(x_2) + \gamma(x_2)\gamma(x_1) = 2x_1 \cdot \nu x_2 \mathbb{1}, \quad x_1, x_2 \in \mathcal{X}, \lambda \in \mathbb{R}.$$

As a *vector space* $\mathrm{Cliff}(\mathcal{X}, \nu)$ is isomorphic to $\wedge\mathcal{X}$.

$\mathrm{Cliff}(\mathcal{X}, \nu)$ has an involutive automorphism α defined by $\alpha(\gamma(x)) = -\gamma(x)$, which defines a $\mathbb{Z}_2$-grading $\mathrm{Cliff}(\mathcal{X}, \nu) = \mathrm{Cliff}_0(\mathcal{X}, \nu) \oplus \mathrm{Cliff}_1(\mathcal{X}, \nu)$. The set $\mathrm{Cliff}_0(\mathcal{X}, \nu)$ of elements of even degree is a sub-algebra of $\mathrm{Cliff}(\mathcal{X}, \nu)$.

The Clifford algebras $\mathrm{Cliff}_{(0)}(\mathbb{R}^{1,d})$ will be simply denoted by $\mathrm{Cliff}_{(0)}(1, d)$.

17.2.1. Volume element. Let $(x_1, \ldots, x_n)$ be an orthonormal basis of $(\mathcal{X}, \nu)$, i.e. such that $x_1 \cdot \nu x_1 = -1$, $x_i \cdot \nu x_i = 1$ for $2 \leq i \leq n$. In particular, this fixes an orientation of $\mathcal{X}$. Set

$$\eta = \gamma(x_1) \cdots \gamma(x_n);$$

η is called the *volume element* and is independent of the choice of the oriented orthonormal basis $(x_1, \ldots, x_n)$. One has

$$\eta\gamma(x) = (-1)^{n+1}\gamma(x)\eta, \quad \eta^2 = \begin{cases} -\mathbb{1}, & \text{if } n \in \{0, 1\} \bmod 4, \\ \mathbb{1}, & \text{if } n \in \{2, 3\} \bmod 4. \end{cases} \tag{17.2}$$

17.2.2. Pseudo-Euclidean group. Each $r \in O(\mathcal{X},\nu)$ induces an automorphism $\hat{r}$ of $\mathrm{Cliff}(\mathcal{X},\nu)$, defined by

$$\hat{r}(\gamma(x)) = \gamma(rx), \quad x \in \mathcal{X}.$$

The map $O(\mathcal{X},\nu) \ni r \mapsto \hat{r} \in Aut(\mathrm{Cliff}(\mathcal{X},\nu))$ is a group morphism. More generally, if $r : (\mathcal{X},\nu) \to \mathbb{R}^{1,d}$ is orthogonal, then it induces an isomorphism $\hat{r} : \mathrm{Cliff}(\mathcal{X},\nu) \to \mathrm{Cliff}(\mathbb{R}^{1,d})$.

17.3. Clifford representations

Let S a complex vector space. A morphism

$$\rho : \mathrm{Cliff}(\mathcal{X},\nu) \longrightarrow L(S)$$

is called a *representation* of $\mathrm{Cliff}(\mathcal{X},\nu)$ in S. It is called *faithful* if it is injective. It is called *irreducible* if $[B,\rho(A)] = 0$ for all $A \in \mathrm{Cliff}(\mathcal{X},\nu)$ implies $B = \lambda \mathbb{1}_S$ for $\lambda \in \mathbb{C}$. We set $\gamma^\rho(x) = \rho(\gamma(x))$ for $x \in \mathcal{X}$. Let $\imath \in \{1, \mathrm{i}\}$ such that

$$\eta^2 = \imath^2 \mathbb{1}, \quad \text{i.e.} \quad \begin{cases} \imath = \mathrm{i}, & \text{if } n \in \{0,1\} \bmod 4, \\ \imath = \mathbb{1}, & \text{if } n \in \{2,3\} \bmod 4. \end{cases} \tag{17.3}$$

Proposition 17.3.1. (1) *Assume that $n = 2m$ is even.*

Then there is a unique up to equivalence, faithful and irreducible representation of $\mathrm{Cliff}(\mathcal{X},\nu)$*, called the* Dirac representation *in a space S of dimension 2^m, whose elements are called* Dirac spinors*. One has $\mathbb{C} \otimes \rho(\mathrm{Cliff}(\mathcal{X},\nu)) = End(S)$.*

Setting $H = \imath\rho(\eta)$, we have $H^2 = \mathbb{1}$ and $[H, \rho(\mathrm{Cliff}_0(\mathcal{X},\nu))] = 0$. Setting $\mathcal{W}_{\mathrm{e/o}} = \{\psi \in S : H\psi = \pm\psi\}$, the representation ρ restricted to $\mathrm{Cliff}_0(\mathcal{X},\nu)$ splits as the direct sum $\rho_+ \oplus \rho_-$ of two irreducible representations on $\mathcal{W}_{\mathrm{e/o}}$. The elements of $\mathcal{W}_{\mathrm{e/o}}$ are called even/odd Weyl spinors*.*

(2) *Assume that $n = 2m+1$ is odd.*

Then there is a unique up to equivalence, faithful and irreducible representation of $\mathrm{Cliff}_0(\mathcal{X},\nu)$*, called the* Pauli representation *in a space S of dimension 2^m, whose elements are called* Pauli spinors*.*

Setting $\rho(\eta) = \imath\mathbb{1}$, the representation of $\mathrm{Cliff}_0(\mathcal{X},\nu)$ *extends to an irreducible representation ρ of* $\mathrm{Cliff}(\mathcal{X},\nu)$ *in S. One has $\mathbb{C} \otimes \rho(\mathrm{Cliff}(\mathcal{X},\nu)) = \mathbb{C} \otimes \rho(\mathrm{Cliff}_0(\mathcal{X},\nu)) = End(S)$.*

The representations $\rho \circ \alpha$ and ρ are not equivalent, and none of them is faithful.

If n is odd then $\eta\mathrm{Cliff}_0(\mathcal{X},\nu) = \mathrm{Cliff}_0(\mathcal{X},\nu)\eta = \mathrm{Cliff}_1(\mathcal{X},\nu)$, which is used in (2) of Proposition 17.3.1 to extend ρ from $\mathrm{Cliff}_0(\mathcal{X},\nu)$ to $\mathrm{Cliff}(\mathcal{X},\nu)$.

In the sequel ρ will denote a representation of $\mathrm{Cliff}(\mathcal{X},\nu)$ as in Proposition 17.3.1, which will be called a *spinor representation*. We have

$$\mathbb{C} \otimes \rho(\mathrm{Cliff}(\mathcal{X},\nu)) = End(S). \tag{17.4}$$

17.3.1. Charge conjugations. Let ρ a spinor representation.

Proposition 17.3.2. (1) *Assume that n is even. Then there exists $\kappa \in End(S_{\mathbb{R}})$ anti-linear such that $\kappa\gamma^\rho(x) = \gamma^\rho(x)\kappa$ and $\kappa^2 = \mathbb{1}$ if $n \in \{2,4\} \bmod 8$, $\kappa^2 = -\mathbb{1}$ if $n \in \{0,6\} \bmod 8$.*

(2) *Assume that n is odd. Then there exists $\kappa \in End(S_{\mathbb{R}})$ anti-linear such that $\kappa\gamma^\rho(x) = (-1)^{(n+1)/2}\gamma^\rho(x)\kappa$ and $\kappa^2 = \mathbb{1}$ if $n \in \{1,3\} \bmod 8$, $\kappa^2 = -\mathbb{1}$ if $n \in \{5,7\} \bmod 8$.*

We refer, e.g. to [**DG**, Theorem 15.19] for the proof. An anti-linear map κ as above is called a *charge conjugation*, with some abuse of terminology if $\kappa^2 = -\mathbb{1}$ (if $\kappa^2 = -\mathbb{1}$, then S becomes a quaternionic vector space).

Later on we will be only interested in the existence of a true charge conjugation, i.e. with $\kappa^2 = \mathbb{1}$, which is the case iff $n \in \{1, 2, 3, 4\}$ mod 8. We have $\kappa\gamma(x) = \gamma(x)\kappa$ iff $n \in \{1, 2, 4\}$ mod 8, $\kappa\gamma(x) = -\gamma(x)\kappa$ iff $n = 3$ mod 8.

If $\kappa, \tilde{\kappa}$ are two such charge conjugations, then $\kappa^{-1}\tilde{\kappa} \in Aut(S)$ (in particular, it is $\mathbb{C}$-linear) and commutes with $\gamma^\rho(x)$ for all $x \in \mathcal{X}$. Since ρ is irreducible, we have $\tilde{\kappa} = \lambda\kappa$, $\lambda \in \mathbb{C}$ and from $\kappa^2 = \tilde{\kappa}^2$ we obtain that $\overline{\lambda}\lambda = 1$.

Let us denote by $C(\rho)$ the set of charge conjugations in Proposition 17.3.2. By the above discussion, we have

$$C(\rho) \sim \mathbb{S}^1, \tag{17.5}$$

or, more pedantically, the group $\mathbb{S}^1$ acts freely and transitively on $C(\rho)$.

17.3.2. Positive energy Hermitian forms.

PROPOSITION 17.3.3. *Let us equip $(\mathcal{X}, \nu)$ with an orientation and a time orientation, so that $(\mathcal{X}, \nu) \sim \mathbb{R}^{1,d}$. Let $\rho : \mathrm{Cliff}(\mathcal{X}, \nu) \to End(S)$ be a spinor representation. Then there exists a Hermitian form $\beta \in L_{\mathrm{h}}(S, S^*)$ such that*

$$\gamma^{\rho *}(x)\beta = -\beta\gamma^\rho(x), \quad x \in \mathcal{X},\ \mathrm{i}\beta\gamma^\rho(e) > 0,$$

for all time-like, future directed $e \in \mathcal{X}$.

Hermitian forms β as above are called *positive energy Hermitian forms*.

Proof. Let us fix a positively oriented orthonormal basis $(e_0, e_1, \ldots, e_n)$ of $(\mathcal{X}, \nu)$ with e_0 time-like and future directed. We set

$$\phi_0 = \mathrm{i}\gamma^\rho(e_0), \quad \phi_j = \gamma^\rho(e_j), \quad 1 \leq j \leq n.$$

From the ϕ_j we obtain an irreducible representation of $\mathrm{Cliff}(\mathbb{R}^n)$, defined as in Definition 17.2.1 with ν replaced by the Euclidean scalar product on $\mathbb{R}^n$. It is well known that one can equip S with a positive definite scalar product $\lambda \in L_{\mathrm{h}}(S, S^*)$ such that $\phi_j = \phi_j^*$ for this scalar product. Setting $\beta = \mathrm{i}\lambda \circ \gamma_0$, we obtain that $\gamma_j^*\beta = -\beta\gamma_j$ and $\mathrm{i}\beta\gamma_0 > 0$. Let now $e \in \mathcal{X}$ be time-like future directed. We can assume that $e \cdot \nu e = -1$, and hence there exists $r \in SO^\uparrow(\mathcal{X}, \nu)$ such that $e = re_0$.

It is well known that there exists an element U of the restricted spin group $\mathrm{Spin}^\uparrow(\mathcal{X}, \nu)$, see Section 17.4, such that $\gamma(rx) = U\gamma(x)U^{-1}$, for $x \in \mathcal{X}$.

Denoting by A^* the adjoint of $A \in End(S)$ for the Hermitian form β, one then checks that $\gamma(rx) = U^*\gamma(x)(U^*)^{-1}$ hence $UU^* = \pm\mathbb{1}$. Since $\mathrm{Spin}^\uparrow(\mathcal{X}, \nu)$ is connected, we have $UU^* = \mathbb{1}$. Now we have $\gamma^\rho(e) = U\gamma^\rho(x_0)U^*$, hence $\mathrm{i}\beta\gamma^\rho(e) > 0$. □

As in Subsection 17.3.1, we denote by $B(\rho)$ the set of positive energy Hermitian forms on S. Then the same argument yields

$$B(\rho) \sim \mathbb{R}^{+*}, \tag{17.6}$$

with the same meaning that the group $\mathbb{R}^{+*}$ acts freely and transitively on $B(\rho)$.

17.4. Spin groups

The *spin group* $\mathrm{Spin}(\mathcal{X}, \nu)$ is the group

$$\mathrm{Spin}(\mathcal{X}, \nu) := \{\gamma(x_1) \cdots \gamma(x_{2p}) : x_i \cdot \nu x_i = \pm 1, p \in \mathbb{N}\} \subset \mathrm{Cliff}(\mathcal{X}, \nu).$$

The *restricted spin group* $\mathrm{Spin}^\uparrow(\mathcal{X}, \nu)$ is the connected component of $\mathbb{1}$ in $\mathrm{Spin}(\mathcal{X}, \nu)$. One can show that $a = \gamma(x_1) \cdots \gamma(x_{2p})$ belongs to $\mathrm{Spin}^\uparrow(\mathcal{X}, \nu)$ iff the number of indices i, $1 \leq i \leq p$, with $x_i \cdot \nu x_i = -1$ is even.

The spin groups $\mathrm{Spin}^{(\uparrow)}(\mathbb{R}^{1,d})$ will be simply denoted by $\mathrm{Spin}^{(\uparrow)}(1,d)$.

If $a \in \mathrm{Spin}^{(\uparrow)}(\mathcal{X},\nu)$, then

$$a\gamma^{\rho}(x)a^{-1} = \gamma^{\rho}(\mathrm{Ad}(a)x), \quad \mathrm{Ad}(a) \in SO^{(\uparrow)}(\mathcal{X},\nu), \tag{17.7}$$

and we have the exact sequence of groups:

$$1 \longrightarrow \mathbb{Z}_2 \longrightarrow \mathrm{Spin}^{(\uparrow)}(\mathcal{X},\nu) \xrightarrow{\mathrm{Ad}} SO^{(\uparrow)}(\mathcal{X},\nu) \longrightarrow 1.$$

Let us fix a spinor representation $\rho_0 : \mathrm{Cliff}(1,d) \to L(S_0)$ (recall that S_0 is a complex vector space of dimension $2^{[n/2]}$). We denote $\rho_0(\gamma(v))$ by $\gamma_0(v)$ for $v \in \mathbb{R}^{1,d}$ and identify $\mathrm{Spin}^{\uparrow}(1,d)$ with its image in $L(S_0)$. We fix a positive energy Hermitian form β_0 and a charge conjugation κ_0 on S_0.

One can show that $\mathrm{Spin}^{\uparrow}(1,d)$ is the set of elements $a \in GL(S_0)$ such that

$$\begin{aligned} &\text{(i)} \quad a^*\beta_0 a = \beta_0, a\kappa_0 = \kappa_0 a, \\ &\text{(ii)} \quad a\gamma_0(v)a^{-1} = \gamma_0(\mathrm{Ad}(a)v),\ \forall v \in \mathbb{R}^{1,d}. \end{aligned} \tag{17.8}$$

This characterization of $\mathrm{Spin}^{\uparrow}(1,d)$ inside $GL(S_0)$ is independent on the choice of β_0, κ_0.

17.5. Weyl bi-spinors

Let us assume that $n = 4$, and let $\rho : \mathrm{Cliff}(\mathcal{X},\nu) \to End(S)$ be a spinor representation, so that $\dim_{\mathbb{C}} S = 4$. To simplify notation, we denote $\rho(A)$ simply by A for $A \in \mathrm{Cliff}(\mathcal{X},\nu)$.

Let κ be a charge conjugation as in Proposition 17.3.2 and let $\beta \in L_{\mathrm{h}}(S,S^*)$ be a positive energy Hermitian form as in Proposition 17.3.3. Recall that

$$\begin{aligned} &\kappa\gamma(x) = \gamma(x)\kappa, \quad \kappa^2 = \mathbb{1}, \\ &\gamma^*(x)\beta = -\beta\gamma(x), \quad \mathrm{i}\beta\gamma(e) > 0 \ \text{ for } e \in \mathcal{X} \text{ future directed time-like.} \end{aligned} \tag{17.9}$$

If η is the volume element we have $\eta^2 = -\mathbb{1}, \eta^*\beta = \beta\eta$, hence $H = \mathrm{i}\eta$ satisfies $H^2 = \mathbb{1}, H^*\beta = -\beta H$. We recall that $S = \mathcal{W}_{\mathrm{e}} \oplus \mathcal{W}_{\mathrm{o}}$ for $\mathcal{W}_{\mathrm{e/o}} = \mathrm{Ker}(H \mp \mathbb{1})$. Since $\kappa\eta = \eta\kappa$ we have $\kappa H = -H\kappa$ hence $\dim_{\mathbb{C}} \mathcal{W}_{\mathrm{e/o}} = 2$ and

$$\kappa : \mathcal{W}_{\mathrm{e/o}} \xrightarrow{\sim} \overline{\mathcal{W}}_{\mathrm{o/e}}. \tag{17.10}$$

We obtain also that

$$\overline{u}_{\mathrm{e/o}} \cdot \beta v_{\mathrm{e/o}} = 0, \quad u_{\mathrm{e/o}}, v_{\mathrm{e/o}} \in \mathcal{W}_{\mathrm{e/o}} \tag{17.11}$$

hence

$$\beta = \mathcal{W}_{\mathrm{e/o}} \xrightarrow{\sim} \mathcal{W}^*_{\mathrm{o/e}}. \tag{17.12}$$

Let $\tilde{\beta} = \kappa^*\beta\kappa \in L_{\mathrm{h}}(S,S^*)$, i.e.

$$\bar{v}_1 \cdot \tilde{\beta} v_2 := \overline{\kappa v}_2 \cdot \beta\kappa v_1, \quad v_1, v_2 \in S.$$

From (17.9) we obtain that $\gamma(x)^*\tilde{\beta} = -\tilde{\beta}\gamma(x)$ for $x \in \mathcal{X}$. Moreover, we have

$$\mathrm{i}\tilde{\beta}\gamma(e) = \mathrm{i}\kappa^*\beta\kappa\gamma(e) = -\kappa^*\mathrm{i}\beta\gamma(e)\kappa < 0,$$

if $e \in \mathcal{X}$ is future directed time-like, using that κ and hence κ^* is anti-linear and that $[\kappa, \gamma(e)] = 0$. Therefore, by (17.6), we have $\tilde{\beta} = \alpha\beta$, $\alpha \in \mathbb{R}^-$. Using that $\kappa^2 = \mathbb{1}$ we obtain that $\alpha^2 = 1$, hence

$$\bar{v}_2 \cdot \beta\kappa v_1 = -\bar{v}_1 \cdot \beta\kappa v_2, \quad v_i \in S. \tag{17.13}$$

17.5.1. Weyl bi-spinors. We know that $S = \mathcal{W}_{\rm e} \oplus \mathcal{W}_{\rm o}$, but we can use β to obtain a different decomposition. We introduce the space of *Weyl spinors*:

$$\mathbb{S} := \mathcal{W}_{\rm e}^*,$$

and identify linearly S with $\mathbb{S}^* \oplus \mathbb{S}'$ by the map

$$S \ni \psi \longmapsto \psi_{\rm e} \oplus \kappa\psi_{\rm o} =: \chi \oplus \phi \in \mathbb{S}^* \oplus \mathbb{S}',$$

where $\psi = \psi_{\rm e} \oplus \psi_{\rm o}$ with $\psi_{\rm e/o} \in \mathcal{W}_{\rm e/o}$. We have $\psi = \chi \oplus \kappa\phi$.

The space $\mathbb{S}$ is canonically equipped with the symplectic form

$$\epsilon := \frac{1}{\sqrt{2}}(\beta\kappa)^{-1} \in L(\mathbb{S}, \mathbb{S}').$$

The fact that ϵ is anti-symmetric follows from (17.13), and $\operatorname{Ker}\epsilon = \{0\}$ since $\operatorname{Ker}\beta = \{0\}$.

17.5.2. Another identification. We can identify $\mathcal{X}$ with $L_{\rm a}(\mathbb{S}^*, \mathbb{S})$ as real vector spaces by

$$\mathcal{X} \ni x \longmapsto \beta\gamma(x) \in L_{\rm a}(\mathcal{W}_{\rm e}, \mathcal{W}_{\rm e}^*). \tag{17.14}$$

This map is injective, since ρ is faithful, and since both spaces have the same dimension, it is bijective. By complexification we obtain an isomorphism

$$T : \mathbb{C}\mathcal{X} \ni z \longmapsto \beta\gamma(z) \in L(\mathcal{W}_{\rm e}, \mathcal{W}_{\rm e}^*) \sim \mathcal{W}_{\rm e}^* \otimes \mathcal{W}_{\rm e}' = \mathbb{S} \otimes \overline{\mathbb{S}}. \tag{17.15}$$

In the next proposition we still denote by $\nu \in L_{\rm s}(\mathbb{C}\mathcal{X}, (\mathbb{C}\mathcal{X})')$ the *bilinear* extension of ν.

Proposition 17.5.1. *The map*

$$T : (\mathbb{C}\mathcal{X}, \nu) \xrightarrow{\sim} (\mathbb{S} \otimes \overline{\mathbb{S}}, \epsilon \otimes \overline{\epsilon}).$$

is an isomorphism, i.e.

$$T' \circ (\epsilon \otimes \overline{\epsilon}) \circ T = \nu. \tag{17.16}$$

Proof. Let $a(x) = \kappa\gamma(x) \in L(\mathcal{W}_{\rm e}, \overline{\mathcal{W}}_{\rm e})$. Since $a(x)^2 = x\nu x\mathbb{1}$, we have $(\det a(x))^2 = (x{\cdot}\nu x)^2$, hence $\det a(x) = \pm x{\cdot}\nu x$, where the sign $\pm$ is independent on x by connectedness. Note also that $a(x) = \sqrt{2}\epsilon \circ \beta\gamma(x)$.

Let $\mathcal{B} = (s_1, s_2)$ be a symplectic basis of $\mathbb{S}$ with $s_1 \cdot \epsilon s_2 = 1$. We denote by $\mathcal{B}'$ the dual basis of $\mathbb{S}'$ and by $\overline{\mathcal{B}}$ the basis $\mathcal{B}$ considered as a basis of $\overline{\mathbb{S}}$. Computing the determinants of $a(x)$, ϵ and $\beta\gamma(x)$ in the above bases, we obtain that $2\det\beta\gamma(x) = 2\det\beta\gamma(x)\det\epsilon = \det a(x) = \pm x{\cdot}\nu x$. Since $\mathrm{i}\beta\gamma(e) > 0$ for $e \in \mathcal{X}$ time-like and future directed, we have $\det\beta\gamma(e) < 0$ so $\det a(e) = e{\cdot}\nu e$ and $\det a(x) = x{\cdot}\nu x$ for all $x \in \mathcal{X}$.

If $[\gamma_{jk}(x)]$ is the matrix of $\beta\gamma(x)$ in $\mathcal{B}', \overline{\mathcal{B}}$, so that $T(x) = \sum_{j,k}\gamma_{jk}(x)\overline{s}_j \otimes s_k$, we check that $\langle T(x)|(\epsilon \otimes \overline{\epsilon})T(x)\rangle = 2\det[\beta\gamma(x)] = \det a(x) = x{\cdot}\nu x$. □

17.6. Clifford and spinor bundles

In this subsection and the next two we will use notions on fiber bundles, recalled in Section 5.1.

Let (M, g) be an orientable and time orientable Lorentzian manifold. After fixing an orientation and a time orientation of M, we can assume that the transition maps o_{ij} of TM, see Subsection 5.1.7, take values in $SO^{\uparrow}(\mathbb{R}^{1,d})$. Equivalently, one can view o_{ij} as the transition maps of the principal bundle $Fr^{\uparrow}_{\rm on}(TM)$ of *oriented and time oriented orthonormal frames* of TM.

DEFINITION 17.6.1. *The* Clifford bundle $Cliff(M,g)$ *is the bundle over* M *with typical fiber* $\mathrm{Cliff}(\mathbb{R}^{1,d})$ *defined by the transition maps* $\hat{o}_{ij} \in Aut(\mathrm{Cliff}(\mathbb{R}^{1,d}))$*, where* $o_{ij} : U_{ij} \to SO^{\uparrow}(\mathbb{R}^{1,d})$ *are the transition maps of* TM*.*

Note that $Cliff(M,g)$ is a bundle of algebras.

DEFINITION 17.6.2. *Let* (M,g) *a Lorentzian manifold. A complex vector bundle* $\mathcal{S} \xrightarrow{\pi} M$ *is a* spinor bundle *over* (M,g) *if there exists a morphism*

$$\rho : Cliff(M,g) \longrightarrow End(\mathcal{S})$$

of bundles of algebras over M *such that for each* $x \in M$ *the map* $\rho_x : \mathrm{Cliff}(T_xM, g_x) \to End(\mathcal{S}_x)$ *is a spinor representation.*

Let us fix a spinor representation $\rho_0 : \mathrm{Cliff}(1,d) \to L(S_0)$, a positive energy Hermitian form β_0 and a charge conjugation κ_0 on S_0 as at the end of Section 17.4.

LEMMA 17.6.3. *Let* $\mathcal{S} \xrightarrow{\pi} M$ *be a spinor bundle over* M*. Then one can assume that its transition maps* $t_{ij} : U_{ij} \to GL(S_0)$ *satisfy:*

$$t_{ij} \circ \rho_0(a) \circ t_{ij}^{-1} = \rho_0(\hat{o}_{ij}(a)),\ a \in \mathrm{Cliff}(1,d) \text{ on } U_{ij}. \tag{17.17}$$

Proof. By Subsections 5.1.2 and 5.1.11, we deduce from the existence of the bundle morphism ρ that there exist $\chi_i : U_i \to Hom(\mathrm{Cliff}(1,d), L(S_0))$ such that

$$t_{ij} \circ \chi_j(a) \circ t_{ij}^{-1} = \chi_i(\hat{o}_{ij}(a)),\ a \in \mathrm{Cliff}(1,d).$$

By irreducibility of the spinor representation, there exists $V_i : U_i \to GL(S_0)$ such that

$$\chi_i(a) = V_i \circ \rho_0(a) \circ V_i^{-1},\ a \in \mathrm{Cliff}(1,d).$$

Let us set $\tilde{t}_{ij} = V_i^{-1} \circ t_{ij} \circ V_j$. We check that $\tilde{t}_{ij}$ satisfy (17.17) and note that changing t_{ij} to $\tilde{t}_{ij}$ corresponds by Subsection 5.1.2 to a vector bundle isomorphism. This completes the proof of the lemma. □

17.6.1. The bundles $B(\rho)$ and $C(\rho)$. Let $B(\rho_0)$, resp. $C(\rho_0)$, the sets of positive energy Hermitian forms, resp. of charge conjugations, associated to ρ_0, see Subsections 17.3.1 and 17.3.2.

DEFINITION 17.6.4. *Let* $\mathcal{S} \xrightarrow{\pi} M$ *be a spinor bundle and* $\rho : Cliff(M,g) \to End(\mathcal{S})$ *the associated morphism.*

The bundle $B(\rho) \xrightarrow{\pi} M$ *is the bundle with typical fiber* $B(\rho_0)$ *and transition maps*

$$\beta \mapsto t_{ij}^{*} \beta t_{ij},\ \beta \in B(\rho_0).$$

The bundle $C(\rho) \xrightarrow{\pi} M$ *is the bundle with typical fiber* $C(\rho_0)$ *and transition maps*

$$\kappa \mapsto t_{ij}^{-1} \kappa t_{ij}, \kappa \in C(\rho_0).$$

Note that using that $t_{ij}^{-1} \gamma_0(v) t_{ij} = \gamma_0(o_{ij} v)$ for $v \in \mathbb{R}^{1,d}$, we obtain that the transition maps above preserve the fibers. By the definition of $B(\rho)$ and $C(\rho)$, we immediately obtain the following proposition.

PROPOSITION 17.6.5. *There exist canonical bundle morphisms*

$$B(\rho) \longrightarrow End(\mathcal{S}, \mathcal{S}^{*}),\ C(\rho) \longrightarrow End(\mathcal{S}, \bar{\mathcal{S}}).$$

From Subsections 17.3.2 and 17.3.1, we see that $B(\rho)$, resp. $C(\rho)$ are principal bundles over M with fiber $\mathbb{R}^{+*}$, resp. $\mathbb{S}^1$. Being principal, these bundles are trivial iff they admit a global section.

REMARK 17.6.6. *Local sections of* $B(\rho)$ *can be pieced together using a partition of unity on* M*, since the set* $B(\rho_0)$ *is convex. Therefore* $B(\rho)$ *is a trivial bundle.*

17.7. Spin structures

Next, let us explain the relationship between spin structures and spinor bundles, following [**T**].

DEFINITION 17.7.1. *A* spin structure *on M is a* $\mathrm{Spin}^{\uparrow}(1,d)$*-principal bundle*

$$Spin(M) \xrightarrow{\pi} M$$

with a bundle map $\chi : Spin(M) \to Fr^{\uparrow}_{\mathrm{on}}(TM)$ such that

$$\forall a \in \mathrm{Spin}^{\uparrow}(1,d),\ q \in Spin(M) \text{ one has } \chi(qa) = \chi(q)\mathrm{Ad}(a). \tag{17.18}$$

We recall that a principal bundle admits a right action of its structure group, see Subsection 5.1.5, which is used in (17.18). If $s_{ij} : U_{ij} \to \mathrm{Spin}^{\uparrow}(1,d)$ are the transition maps of $Spin(M)$ and $o_{ij} : U_{ij} \to SO^{\uparrow}(1,d)$ are the transition maps of $Fr^{\uparrow}_{\mathrm{on}}(TM)$, (17.18) means that

$$o_{ij}(x) = \mathrm{Ad}(s_{ij})(x), \quad x \in U_{ij}.$$

THEOREM 17.7.2. *Let (M,g) be an orientable and time-orientable Lorentzian manifold and let $Spin(M) \xrightarrow{\pi} M$ be a spin structure over (M,g). Then there exists a canonical spinor bundle $\mathcal{S} \xrightarrow{\pi} M$ with canonical global sections β, κ of the bundles $B(\rho), C(\rho)$.*

REMARK 17.7.3. *Conversely, one can show that if $\mathcal{S} \xrightarrow{\pi} M$ is a spinor bundle over (M,g) such that the bundle $C(\rho)$ is trivial, then M admits a spin structure $Spin(M) \xrightarrow{\pi} M$. The two constructions are inverse to one another, modulo bundle isomorphisms.*

Proof. Recall that $s_{ij} : U_{ij} \to \mathrm{Spin}^{\uparrow}(1,d)$ are the transition maps of $Spin(M)$. Let $\mathcal{S} \xrightarrow{\pi} M$ be the vector bundle with typical fiber S_0 and transition maps

$$t_{ij} = \rho_0(s_{ij}) : U_{ij} \to GL(S_0).$$

We define the bundle morphism $\rho : Cliff(M,g) \to End(\mathcal{S})$ by

$$\rho_i = \rho_0 : U_i \to Hom(\mathrm{Cliff}(1,d), L(S_0)),$$

see Subsection 5.1.2. From (17.8) (ii), we obtain that ρ is indeed a morphism of bundles of algebras, ie that $\mathcal{S}$ is a spinor bundle over M.

From (17.8) (i) and the definition of t_{ij}, we see that the local sections of $B(\rho)$, resp. $C(\rho)$ defined by $\beta_i(x) = \beta_0$, resp. $\kappa_i(x) = \kappa_0$ for $x \in U_i$ can be patched together as global sections of $B(\rho)$, resp. $C(\rho)$. This completes the proof of the theorem. □

17.8. Spinor connections

Let ∇ be the Levi-Civita connection on (M,g). Since $Cliff(M,g)$ is a vector sub-bundle of $\bigoplus_{k=0}^{n} \otimes^k TM$, ∇ induces a unique connection ∇^{Cl}, defined by

$$\nabla^{Cl}_X \gamma(Y) = \gamma(\nabla_X Y),\ X, Y \in C^{\infty}(M; TM).$$

Since ∇ is metric for g, ∇^{Cl} is adapted to the algebra structure of $Cliff(M,g)$, i.e.

$$\nabla^{Cl}_X(\gamma(Y_1)\gamma(Y_2)) = \nabla^{Cl}_X \gamma(Y_1)\gamma(Y_2) + \gamma(Y_1)\nabla^{Cl}_X \gamma(Y_2).$$

Let now $\mathcal{S} \xrightarrow{\pi} M$ be a spinor bundle and let us denote $\rho(\gamma(X))$ simply by $\gamma(X)$ for X a vector field on M. One can show, see [**T**], that there exists a (non unique) connection $\nabla^{\mathcal{S}}$ on $\mathcal{S}$ such that

$$\nabla^{\mathcal{S}}_X(\gamma(Y)\psi) = \gamma(\nabla_X Y)\psi + \gamma(Y)\nabla^{\mathcal{S}}_X \psi,\ X, Y \in C^{\infty}(M; TM), \psi \in C^{\infty}(M; \mathcal{S}).$$

The following result is shown in [**T**, Proposition 9].

THEOREM 17.8.1. *Let $\mathcal{S} \xrightarrow{\pi} M$ a spinor bundle. Assume that the bundle $C(\rho)$ is trivial. Then given a section $\beta \in C^\infty(M; B(\rho))$ and a section $\kappa \in C^\infty(M; C(\rho))$, there exists a unique connection $\nabla^{\mathcal{S}}$ on $\mathcal{S}$ such that*

$$\begin{aligned} &\text{(i) } \nabla^{\mathcal{S}}_X(\gamma(Y)\psi) = \gamma(\nabla_X Y)\psi + \gamma(Y)\nabla^{\mathcal{S}}_X\psi, \\ &\text{(ii) } X((\psi|\beta\psi)) = (\nabla^{\mathcal{S}}_X\psi|\beta\psi) + (\psi|\beta\nabla^{\mathcal{S}}_X\psi), \\ &\text{(iii) } \nabla^{\mathcal{S}}_X(\kappa\psi) = \kappa\nabla^{\mathcal{S}}_X\psi, \end{aligned} \tag{17.19}$$

for all $X, Y \in C^\infty(M; TM)$ and $\psi \in C^\infty(M; \mathcal{S})$.

From Theorem 17.7.2 we see that if $Spin(M) \xrightarrow{\pi} M$ is a spin structure over M, then there exists a canonical spinor bundle $\mathcal{S} \xrightarrow{\pi} M$, canonical sections β, κ and spin connection $\nabla^{\mathcal{S}}$.

17.9. Dirac operators

In the rest of this chapter we will assume that the hypotheses of Theorem 17.8.1 are satisfied. One defines a *Dirac operator*, acting on smooth sections of $\mathcal{S}$ as follows:

let $U \subset M$ a chart open set for $\mathcal{S}$ and the bundle of frames $Fr(TM)$. Choose sections e_μ, $1 \le \mu \le n$ of $Fr(TM)$ over U, i.e. $(e_1(x), \cdots e_n(x))$ is a ordered basis of T_xM for $x \in M$ (not necessarily orthogonal). We define

$$\begin{aligned} \not{D} &= g^{\mu\nu}\gamma(e_\mu)\nabla^{\mathcal{S}}_{e_\nu}, \\ D &= \not{D} + m(x) \end{aligned} \tag{17.20}$$

where $\nabla^{\mathcal{S}}$ is the connection on $\mathcal{S}$ from Theorem 17.8.1 and $m \in C^\infty(M; End(\mathcal{S}))$ is such that $m^*\beta = \beta m$ where β is the section of $B(\rho)$ in Theorem 17.8.1. Such an operator will be called a *Dirac operator*.

17.9.1. Characteristic manifold. Denoting by $X = (x, \xi)$ the elements of $T^*M \setminus o$, the *principal symbol* $d(x, \xi)$ of D is the section of $C^\infty(T^*M \setminus o; End(\mathcal{S}))$, homogeneous of degree 1 in ξ, given by

$$d(x, \xi) = \gamma(g^{-1}(x)\xi).$$

From the Clifford relations we obtain that

$$d^2(x, \xi) = \xi \cdot g^{-1}(x)\xi \mathbb{1}. \tag{17.21}$$

The characteristic manifold of D is

$$\mathrm{Char}(D) := \{(x, \xi) \in T^*M \setminus o : d(x, \xi) \text{ is not invertible}\},$$

and by (17.21) we have

$$\mathrm{Char}(D) = \{(x, \xi) \in T^*M \setminus o : \xi \cdot g^{-1}(x)\xi = 0\} = \mathcal{N}.$$

As usual, we denote by $\mathcal{N}^\pm$ the two connected components of $\mathcal{N}$.

17.9.2. Charge conjugation. Assume that the charge conjugation κ satisfies $\kappa^2 = \mathbb{1}$, i.e. that $n \in \{1, 2, 3, 4\}$ mod 8 by Proposition 17.3.2. By (17.19), we have $[\kappa, \nabla^{\mathcal{S}}_X] = 0$. Assuming also that m is *real*, i.e. $[m, \kappa] = 0$, we obtain that

$$\begin{aligned} &D\kappa = \kappa D \quad \text{if } n \in \{1, 2, 4\} \text{ mod } 8, \\ &D\kappa = -\kappa D \quad \text{if } n = 3 \text{ mod } 8 \text{ and } m = 0. \end{aligned}$$

17.9.3. Conserved current. Let $\psi_1, \psi_2 \in C^\infty(M;S)$. Define the 1-form $J(\psi_1,\psi_2) \in C^\infty(M;T^*M)$ by

$$J(\psi_1,\psi_2)\cdot X := \overline{\psi}_1 \cdot \beta\gamma(X)\psi_2, \quad X \in C^\infty(M;TM).$$

The following lemma follows easily from (17.19).

LEMMA 17.9.1. *We have*

$$\nabla^\mu J_\mu(\psi_1,\psi_2) = -\overline{D\psi_1}\cdot\beta\psi_2 + \overline{\psi}_1\cdot\beta D\psi_2, \quad \psi_i \in C^\infty(M;\mathcal{S}).$$

PROPOSITION 17.9.2. *The Dirac operator D is formally selfadjoint on $C_0^\infty(M;\mathcal{S})$ with respect to the Hermitian form*

$$(\psi_1|\psi_2)_M := \int_M \overline{\psi}_1\cdot\beta\psi_2 \, dVol_g. \tag{17.22}$$

Proof. We apply the identity $\nabla^\mu J_\mu \Omega_g = d(J^\mu \lrcorner \Omega_g)$, where Ω_g is the volume form on (M,g), and the Stokes formula (5.11) $\int_U d\omega = \int_{\partial U}\omega$ to $\omega = J^\mu \lrcorner \Omega_g$, $U \Subset M$ an open set with smooth boundary, containing $\operatorname{supp}\psi_i$. □

17.9.4. Decomposition of the Dirac operator. Let us assume that $n=4$ and that m in (17.20) is scalar, i.e. $m(x) = m(x)\mathbb{1}$ for $m \in C^\infty(M;\mathbb{R})$.

Section 17.5 provides a section $H \in C^\infty(M;End(\mathcal{S}))$ locally defined by $H = \mathrm{i}\gamma(e_1)\cdots\gamma(e_4)$, where $(e_1,\dots,e_4)$ is an oriented orthonormal frame of TM. We have

$$H^2 = \mathbb{1}, \quad H\gamma(X) = -\gamma(X)H, \quad X \in C^\infty(M;TM).$$

Using (17.19), the fact that ∇ is metric for g, and the Clifford relations, one can prove that $\nabla^{Cl}H = 0$, which implies that $\not{D}H = -H\not{D}$.

Using $P_{\mathrm{e/o}} = \frac{1}{2}(1 \pm H)$, we can construct the vector bundles $\mathcal{W}_{\mathrm{e/o}} = P_{\mathrm{e/o}}S$ and identify $C^\infty(M;\mathcal{S})$ with $C^\infty(M;\mathcal{W}_{\mathrm{e}}) \oplus C^\infty(M;\mathcal{W}_{\mathrm{o}})$. The Dirac operator becomes

$$D = \begin{pmatrix} m & \not{D}_{\mathrm{o}} \\ \not{D}_{\mathrm{e}} & m \end{pmatrix}, \quad \text{with } \not{D}_{\mathrm{e/o}} = (g^{\mu\nu}\gamma(e_\mu)\nabla_{e_\nu})\restriction_{C^\infty(M;\mathcal{W}_{\mathrm{e/o}})}. \tag{17.23}$$

By Subsection 17.9.2, there exists a charge conjugation κ with $\kappa^2 = \mathbb{1}$ and $D\kappa = \kappa D$, $\kappa : \mathcal{W}_{\mathrm{e/o}} \xrightarrow{\sim} \overline{\mathcal{W}}_{\mathrm{o/e}}$, and we obtain that

$$\not{D}_{\mathrm{e/o}} = \kappa \not{D}_{\mathrm{o/e}} \kappa. \tag{17.24}$$

As in Subsection 17.5.1, we identify $S \xrightarrow{\pi} M$ with $\mathbb{S}^* \oplus \mathbb{S}' \xrightarrow{\pi} M$ and a section $\psi \in C^\infty(M;S)$ with $(\chi,\phi) \in C^\infty(M;\mathbb{S}^*) \oplus C^\infty(M;\mathbb{S}')$. We can rewrite the Dirac equation

$$\not{D}\psi + m\psi = 0$$

as

$$\begin{cases} \beta\not{D}\chi + \frac{m}{\sqrt{2}}\epsilon^{-1}\phi = 0, \\ \kappa'\beta\not{D}\kappa\phi + \frac{m}{\sqrt{2}}\bar{\epsilon}^{-1}\chi = 0. \end{cases} \tag{17.25}$$

17.10. Dirac equation on globally hyperbolic spacetimes

Assume now that (M,g) is a globally hyperbolic spacetime. We denote by $\mathrm{Sol}_{\mathrm{sc}}(D)$ the space of smooth, space compact solutions of the Dirac equation

$$D\psi = 0.$$

17.10.1. Retarded/advanced inverses. Since (M, g) is globally hyperbolic, D admits unique *retarded/advanced inverses* $G_{\mathrm{ret/adv}} : C_0^\infty(M;\mathcal{S}) \to C_{\mathrm{sc}}^\infty(M;\mathcal{S})$ such that

$$\begin{cases} DG_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}}D = \mathbb{1}, \\ \operatorname{supp} G_{\mathrm{ret/adv}}u \subset J_\pm(\operatorname{supp} u), \quad u \in C_0^\infty(M;\mathcal{S}), \end{cases}$$

see eg [**DG**, Theorem 19.61]. Using the fact that D is formally selfadjoint with respect to $(\cdot|\cdot)_M$ and the uniqueness of $G_{\mathrm{ret/adv}}$ we obtain that

$$G_{\mathrm{ret/adv}}^* = G_{\mathrm{adv/ret}},$$

where the adjoint is computed with respect to $(\cdot|\cdot)_M$. Therefore, the *causal propagator*

$$G := G_{\mathrm{ret}} - G_{\mathrm{adv}}$$

satisfies

$$\begin{cases} DG = GD = 0, \\ \operatorname{supp} Gu \subset J(\operatorname{supp} u), \quad u \in C_0^\infty(M;\mathcal{S}), \\ G^* = -G. \end{cases} \tag{17.26}$$

17.10.2. The Cauchy problem. Let $\Sigma \subset M$ be a smooth, space-like Cauchy surface and denote by n its future directed unit normal and by $\mathcal{S}_\Sigma$ the restriction of the spinor bundle $\mathcal{S}$ to Σ, so that

$$\rho_\Sigma : C^\infty(M;\mathcal{S}) \ni \psi \longmapsto \psi\restriction_\Sigma \in C^\infty(\Sigma;\mathcal{S}_\Sigma)$$

is surjective. The Cauchy problem

$$\begin{cases} D\psi = 0, \\ \rho_\Sigma\psi = f, \quad f \in C_0^\infty(\Sigma;\mathcal{S}_\Sigma), \end{cases}$$

is globally well-posed, the solution being denoted by $\psi = U_\Sigma f$. From [**DG**, Theorem 19.63], we obtain that

$$U_\Sigma f(x) = -\int_\Sigma G(x,y)\gamma(n(y))f(y)dVol_h, \tag{17.27}$$

where h is the Riemannian metric induced by g on Σ.

We equip $C_0^\infty(\Sigma;\mathcal{S}_\Sigma)$ with the Hermitian form

$$(f_1|f_2)_\Sigma := \int_\Sigma \overline{f}_1 \cdot \beta f_2 \, dVol_h. \tag{17.28}$$

For $g \in \mathcal{E}'(\Sigma;\mathcal{S}_\Sigma)$, we define $\rho_\Sigma^* g \in \mathcal{D}'(M;\mathcal{S})$ by

$$\int_M \overline{\rho_\Sigma^* g} \cdot \beta u \, dVol_g := \int_\Sigma \overline{g} \cdot \beta \rho_\Sigma u dVol_h, \ u \in C^\infty(\Sigma;\mathcal{S}_\Sigma),$$

i.e. ρ_Σ^* is the adjoint of ρ_Σ with respect to the scalar products $(\cdot|\cdot)_M$ and $(\cdot|\cdot)_\Sigma$. We can rewrite (17.27) as

$$U_\Sigma f = (\rho_\Sigma G)^* \gamma(n) f, \quad f \in C_0^\infty(\Sigma;\mathcal{S}_\Sigma). \tag{17.29}$$

17.11. Quantization of the Dirac equation

For $\psi_1, \psi_2 \in \mathrm{Sol}_{\mathrm{sc}}(D)$ we set

$$\overline{\psi}_1 \cdot \nu \psi_2 := \int_\Sigma \mathrm{i} J_\mu(\psi_1, \psi_2) n^\mu dVol_h = (\rho_\Sigma \psi_1 | \mathrm{i}\gamma(n)\rho_\Sigma \psi_2)_\Sigma. \tag{17.30}$$

Since $\nabla^\mu J_\mu(\psi_1, \psi_2) = 0$, the right-hand side of (17.28) is independent on the choice of Σ, and ν is a positive definite scalar product on $\mathrm{Sol}_{\mathrm{sc}}(D)$. Setting

$$\overline{f}_1 \cdot \nu_\Sigma f_2 := \mathrm{i} \int_\Sigma \overline{f}_1 \cdot \beta\gamma(n) f_2 dVol_h,$$

we obtain that

$$\rho_\Sigma : (\mathrm{Sol}_{\mathrm{sc}}(D), \nu) \to (C_0^\infty(\Sigma; \mathcal{S}_\Sigma), \nu_\Sigma)$$

is unitary, with inverse U_Σ. We also get that $G : C_0^\infty(M; \mathcal{S}) \to \mathrm{Sol}_{\mathrm{sc}}(D)$ is surjective with kernel $DC_0^\infty(M; \mathcal{S})$ and, see e.g. [**DG**, Theorem 19.65], that

$$G : (\frac{C_0^\infty(M; \mathcal{S})}{DC_0^\infty(M; \mathcal{S})}, \mathrm{i}(\cdot | G \cdot)_M) \to (\mathrm{Sol}_{\mathrm{sc}}(D), \nu)$$

is unitary. Summarizing, the maps

$$(\tfrac{C_0^\infty(M;\mathcal{S})}{DC_0^\infty(M;\mathcal{S})}, \mathrm{i}(\cdot|G\cdot)_M) \xrightarrow{G} (\mathrm{Sol}_{\mathrm{sc}}(D), \nu) \xrightarrow{\rho_\Sigma} (C_0^\infty(\Sigma; \mathcal{S}_\Sigma), \nu_\Sigma) \tag{17.31}$$

are unitary.

17.12. Hadamard states for the Dirac equation

We denote by $\mathrm{CAR}(D)$ the $*$-algebra $\mathrm{CAR}(\mathcal{Y}, \nu)$ for $(\mathcal{Y}, \nu)$ one of the equivalent pre-Hilbert spaces in (17.31). We use the Hermitian form $(\cdot|\cdot)_M$ in (17.22) to pair $C_0^\infty(M; \mathcal{S})$ with $\mathcal{D}'(M; \mathcal{S})$ and to identify continuous sesquilinear forms on $C_0^\infty(M; \mathcal{S})$ with continuous linear maps from $C_0^\infty(M; \mathcal{S})$ to $\mathcal{D}'(M; \mathcal{S})$.

Thus, a quasi-free state ω on $\mathrm{CAR}(D)$ is defined by its *spacetime covariances* $\Lambda^\pm$ which satisfy

$$\begin{aligned}
&\text{(i)} \quad \Lambda^\pm : C_0^\infty(M; \mathcal{S}) \to \mathcal{D}'(M; \mathcal{S}) \text{ are linear continuous,} \\
&\text{(ii)} \quad \Lambda^\pm \geq 0 \text{ with respect to } (\cdot|\cdot)_M, \\
&\text{(iii)} \quad \Lambda^+ + \Lambda^- = \mathrm{i}G, \\
&\text{(iv)} \quad D \circ \Lambda^\pm = \Lambda^\pm \circ D = 0.
\end{aligned} \tag{17.32}$$

Alternatively, one can define ω by its Cauchy surface covariances $\lambda_\Sigma^\pm$, which satisfy

$$\begin{aligned}
&\text{(i)} \quad \lambda_\Sigma^\pm : C_0^\infty(\Sigma; \mathcal{S}_\Sigma) \to \mathcal{D}'(\Sigma; \mathcal{S}_\Sigma) \text{ are linear continuous,} \\
&\text{(ii)} \quad \lambda_\Sigma^\pm \geq 0 \text{ for } (\cdot|\cdot)_\Sigma, \\
&\text{(iii)} \quad \lambda_\Sigma^+ + \lambda_\Sigma^- = \mathrm{i}\gamma(n).
\end{aligned} \tag{17.33}$$

Using (17.29) one can show as in Proposition 6.1.6 that

$$\begin{aligned}
\Lambda^\pm &= (\rho_\Sigma G)^* \lambda_\Sigma^\pm (\rho_\Sigma G), \\
\lambda_\Sigma^\pm &= (\rho_\Sigma^* \gamma(n))^* \Lambda^\pm (\rho_\Sigma^* \gamma(n)).
\end{aligned} \tag{17.34}$$

By the Schwartz kernel theorem, we can identify $\Lambda^\pm$ with distributional sections in $\mathcal{D}'(M \times M; \mathcal{S} \boxtimes \mathcal{S})$, still denoted by $\Lambda^\pm$.

The wavefront set of such sections is defined in the natural way: choosing a local trivialization of $\mathcal{S} \boxtimes \mathcal{S}$, one can assume that $\mathcal{S} \boxtimes \mathcal{S}$ is trivial with fiber $M_p(\mathbb{C})$ for $p = \operatorname{rank} \mathcal{S}$, and the wavefront set of a matrix valued distribution is simply the union of the wavefront sets of its entries.

We recall that $\mathcal{N}^\pm$ are the two connected components of $\mathcal{N}$, see 17.9.1.

DEFINITION 17.12.1. *ω is a Hadamard state if*

$$\mathrm{WF}(\Lambda^{\pm}) \subset \mathcal{N}^{\pm} \times \mathcal{N}^{\pm}.$$

The following version of Proposition 11.1.1 gives a sufficient condition for the Cauchy surface covariances $\lambda_{\Sigma}^{\pm}$ to generate a Hadamard state. Its proof is analogous, using (17.34).

PROPOSITION 17.12.2. *Let $\lambda_{\Sigma}^{\pm} =: \mathrm{i}\gamma(n)c^{\pm}$, where $c^{\pm}$ are linear continuous from $C_0^{\infty}(\Sigma; \mathcal{S}_{\Sigma})$ to $C^{\infty}(\Sigma; \mathcal{S}_{\Sigma})$ and from $\mathcal{E}'(\Sigma; \mathcal{S}_{\Sigma})$ to $\mathcal{D}'(\Sigma; \mathcal{S}_{\Sigma})$. Assume that*

$$\mathrm{WF}(U_{\Sigma} \circ c^{\pm})' \subset \mathcal{N}^{\pm} \times (T^*\Sigma \setminus o), \ \text{over } U \times \Sigma,$$

for some neighborhood U of Σ in M. Then ω is a Hadamard state.

The existence of Hadamard states for Dirac equations on globally hyperbolic spacetimes can be shown by the same deformation argument as in the Klein-Gordon case, see e.g. [**Ho1**].

17.13. Conformal transformations

Let $c \in C^{\infty}(M)$ with $c(x) > 0$ and $\tilde{g} = c^2 g$. If $\tilde{\gamma}(X)$ are the generators of $Cliff(M, \tilde{g})$, we have $\tilde{\gamma}(X) = c\gamma(X)$.

To define the spinor connection $\widetilde{\nabla}^{\mathcal{S}}$ on S for the metric $\tilde{g}$ we need to fix a Hermitian form $\tilde{\beta}$ and a charge conjugation $\tilde{\kappa}$. It is natural to choose $\tilde{\kappa} = \kappa$, but several choices of $\tilde{\beta}$ are possible. The choice that we will adopt is

$$\tilde{\beta} = c^{-1}\beta$$

which has the advantage that if $n = 4$ the isomorphism T in Proposition 17.5.1 is unchanged. From Theorem 17.8.1 we deduce that

$$\widetilde{\nabla}_X^{\mathcal{S}} = \nabla_X^{\mathcal{S}} + \frac{1}{2}c^{-1}\gamma(X)\gamma(\nabla c) - c^{-1}X \cdot dc \, \mathbb{1}.$$

If $\tilde{\not{D}}$ is the associated Dirac operator, we have

$$\tilde{\not{D}} = c^{-n/2} \not{D} c^{n/2-1}. \tag{17.35}$$

Equivalently, if we introduce the map

$$W : C_0^{\infty}(M; \mathcal{S}) \ni \tilde{\psi} \longmapsto c^{n/2-1}\tilde{\psi} \in C_0^{\infty}(M; \mathcal{S}),$$

and denote by $(\cdot|\cdot)_{\tilde{M}}$ the Hermitian form (17.22) with β and $dVol_g$ replaced by $\tilde{\beta}$ and $dVol_{\tilde{g}}$, respectively, we have

$$(\psi_1 | W\tilde{\psi}_2)_M = (W^*\psi_1 | \tilde{\psi}_2)_{\tilde{M}}, \quad W^*\psi = c^{-n/2}\psi, \tag{17.36}$$

and (17.35) can be rewritten as:

$$\tilde{D} := W^* D W = c^{-n/2} D c^{n/2-1} = \tilde{\not{D}} + c^{-1}m.$$

We have then $G = W\tilde{G}W^*$.

REMARK 17.13.1. *The choice $\tilde{\beta} = \beta$ is often used in the mathematics literature. It leads to*

$$\widetilde{\nabla}_X^{\mathcal{S}} = \nabla_X^{\mathcal{S}} + \tfrac{1}{2}c^{-1}\gamma(X)\gamma(\nabla c) - \tfrac{1}{2}c^{-1}X \cdot dc \, \mathbb{1},$$
$$\tilde{\not{D}} = c^{-(n+1)/2} \not{D} c^{(n-1)/2}.$$

17.13.1. Conformal transformations of phase spaces. Setting

$$U : C_0^\infty(\Sigma; \mathcal{S}_\Sigma) \ni f \longmapsto Uf = c^{1-n/2} f \ni C_0^\infty(\Sigma; \mathcal{S}_\Sigma),$$

we obtain the following analog of Proposition 6.3.1.

PROPOSITION 17.13.2. *The following diagram is commutative, with all arrows unitary:*

$$\begin{array}{ccccc} (\frac{C_0^\infty(M;\mathcal{S})}{DC_0^\infty(M;\mathcal{S})}, (\cdot\,|\mathrm{i}G\,\cdot)_M) & \xrightarrow{G} & (\mathrm{Sol}_{\mathrm{sc}}(D), \nu) & \xrightarrow{\varrho_\Sigma} & (C_0^\infty(\Sigma; \mathcal{S}_\Sigma), \nu_\Sigma) \\ \downarrow W^* & & \downarrow W^{-1} & & \downarrow U \\ (\frac{C_0^\infty(\tilde{M};\mathcal{S})}{\tilde{D}C_0^\infty(\tilde{M};\mathcal{S})}, (\cdot\,|\mathrm{i}\tilde{G}\,\cdot)_{\tilde{M}}) & \xrightarrow{\tilde{G}} & (\mathrm{Sol}_{\mathrm{sc}}(\tilde{D}), \tilde{\nu}) & \xrightarrow{\tilde{\varrho}_\Sigma} & (C_0^\infty(\Sigma; \mathcal{S}_\Sigma), \tilde{\nu}_\Sigma) \end{array}$$

17.13.2. Conformal transformations of quasi-free states. Let $\Lambda^\pm$ be the spacetime covariances of a quasi-free state ω for D. Then

$$\tilde{\Lambda}^\pm = c^{1-n/2} \Lambda^\pm c^{n/2} \tag{17.37}$$

are the spacetime covariances of a quasi-free state $\tilde{\omega}$ for $\tilde{D}$, and

$$\tilde{\lambda}_\Sigma^\pm = (U^*)^{-1} \lambda_\Sigma^\pm U^{-1} = c^{1-n/2} \lambda_\Sigma^\pm c^{n/2-1},$$

if $\lambda_\Sigma^\pm$, resp. $\tilde{\lambda}_\Sigma^\pm$ are the Cauchy surface covariances of ω, resp. $\tilde{\omega}$.

17.14. The Weyl equation

We consider now the *massless* Dirac equation $\not{D}\psi = 0$ and assume $n = 4$. According to 17.9.4, the Dirac equation decouples as two independent *Weyl equations*

$$\begin{cases} \beta \not{D} \chi = 0, \\ \kappa' \beta \not{D} \kappa \phi = 0. \end{cases} \tag{17.38}$$

Let us set

$$\mathbb{D} := \beta \not{D} : C^\infty(M; \mathbb{S}^*) \longrightarrow C^\infty(M; \mathbb{S}).$$

Note that $\mathbb{D} = \mathbb{D}^*$ by Proposition 17.9.2.

17.14.1. Characteristic manifold. The characteristic manifold of $\mathbb{D}$ is

$$\mathrm{Char}(\mathbb{D}) = \{(x, \xi) \in T^*M \setminus o : \sigma_{\mathrm{pr}}(\mathbb{D})(x, \xi) \text{ not invertible}\}.$$

It is easy to see that

$$\mathrm{Char}(\mathbb{D}) = \mathcal{N}. \tag{17.39}$$

Indeed, fix $x \in M$ and choose a basis (w_1, w_2) of $\mathcal{W}_{\mathrm{e}x}$. By (17.23), the matrix of $d(x, \xi)$ in the basis $(w_1, w_2, \kappa w_1, \kappa w_2)$ of $\mathcal{S}_x$ equals $\begin{pmatrix} 0 & d_{\mathrm{e}}(x, \xi) \\ d_{\mathrm{e}}(x, \xi) & 0 \end{pmatrix}$, where $d_{\mathrm{e}}(x, \xi) \in M_2(\mathbb{R})$. From (17.21) we obtain that $d_{\mathrm{e}}(x, \xi)^2 = \xi \cdot g^{-1}(x) \xi \mathbb{1}_2$, which implies (17.39).

17.14.2. Retarded/advanced inverses. $\mathbb{D}$ has the retarded/advanced inverses

$$\mathbb{G}_{\mathrm{ret/adv}} = G_{\mathrm{ret/adv}} \beta^{-1} : C_0^\infty(M; \mathbb{S}) \longrightarrow C_{\mathrm{sc}}^\infty(M; \mathbb{S}^*),$$

and the causal propagator

$$\mathbb{G} := \mathbb{G}_{\mathrm{ret}} - \mathbb{G}_{\mathrm{adv}} = G \beta^{-1}.$$

Let us denote by $r_\Sigma : C^\infty(M; \mathbb{S}^*) \to C^\infty(\Sigma; \mathbb{S}_\Sigma^*)$ the trace on Σ, and by $r_\Sigma^* : C^\infty(\Sigma; \mathbb{S}_\Sigma) \to C^\infty(M; \mathbb{S})$ its adjoint, so that $r_\Sigma^* = \beta \rho_\Sigma^* \beta^{-1}$. We also set

$$\Gamma(X) = \beta \gamma(X) : C^\infty(\Sigma, \mathbb{S}_\Sigma^*) \longrightarrow C^\infty(\Sigma; \mathbb{S}_\Sigma).$$

The Cauchy problem

$$\begin{cases} \mathbb{D}\phi = 0, \\ r_\Sigma \phi = f \in C_0^\infty(\Sigma; \mathbb{S}^*_\Sigma), \end{cases}$$

has the unique solution

$$\phi = \mathbb{U}_\Sigma f = -\int_\Sigma \mathbb{G}(x,y)\Gamma(n(y))f(y)dVol_h,$$

or equivalently

$$\mathbb{U}_\Sigma = (r_\Sigma \mathbb{G})^* \Gamma(n).$$

We see that $(\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}), \nu)$ is a pre-Hilbert space, and from (17.31) we obtain the unitary maps:

$$(\frac{C_0^\infty(M;\mathbb{S})}{\mathbb{D}C_0^\infty(M;\mathbb{S}^*)}, \mathrm{i}\mathbb{G}) \xrightarrow{\mathbb{G}} (\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}), \nu) \xrightarrow{r_\Sigma} (C_0^\infty(\Sigma; \mathbb{S}^*_\Sigma), \nu_\Sigma). \tag{17.40}$$

17.14.3. Quasi-free states. As before, we denote by $\mathrm{CAR}(\mathbb{D})$ the $*$-algebra $\mathrm{CAR}(\mathcal{Y}, \nu)$ for $(\mathcal{Y}, \nu)$ one of the equivalent pre-Hilbert spaces in (17.40). A quasi-free state ω on $\mathrm{CAR}(\mathcal{Y}, \nu)$ is defined by its spacetime covariances $\mathbb{L}^\pm$, which satisfy

$$\begin{aligned} &\text{(i)} \quad \mathbb{L}^\pm : C_0^\infty(M;\mathbb{S}) \to \mathcal{D}'(M;\mathbb{S}^*) \text{ are linear continuous,} \\ &\text{(ii)} \quad \mathbb{L}^\pm \geq 0, \\ &\text{(iii)} \quad \mathbb{L}^+ + \mathbb{L}^- = \mathrm{i}\mathbb{G}, \\ &\text{(iv)} \quad \mathbb{D}\mathbb{L}^\pm = \mathbb{L}^\pm \mathbb{D} = 0. \end{aligned} \tag{17.41}$$

Alternatively, one can define ω by its Cauchy surface covariances $l^\pm_\Sigma$ which satisfy:

$$\begin{aligned} &\text{(i)} \quad l^\pm_\Sigma : C_0^\infty(\Sigma; \mathbb{S}^*_\Sigma) \to \mathcal{D}'(\Sigma; \mathbb{S}_\Sigma) \text{ are linear continuous,} \\ &\text{(ii)} \quad l^\pm_\Sigma \geq 0, \\ &\text{(iii)} \quad l^+_\Sigma + l^-_\Sigma = \mathrm{i}\Gamma(n). \end{aligned} \tag{17.42}$$

One has

$$\begin{aligned} \mathbb{L}^\pm &= (r_\Sigma \mathbb{G})^* l^\pm_\Sigma (r_\Sigma \mathbb{G}), \\ l^\pm_\Sigma &= (r^*_\Sigma \Gamma(n))^* \mathbb{L}^\pm (r^*_\Sigma \Gamma(n)). \end{aligned} \tag{17.43}$$

Here are the identities corresponding to those in Section 17.13, obtained by a conformal transformation $\tilde{g} = c^2 g$:

$$\begin{aligned} &\tilde{\mathbb{D}} = c^{-1-n/2} \mathbb{D} c^{n/2-1}, \ \tilde{\mathbb{G}} = c^{1-n/2} \mathbb{G} c^{n/2+1}, \\ &\tilde{\mathbb{L}}^\pm = c^{1-n/2} \mathbb{L}^\pm c^{n/2+1}, \ \tilde{l}^\pm_\Sigma = c^{1-n/2} l^\pm_\Sigma c^{n/2-1}. \end{aligned} \tag{17.44}$$

Definition 17.14.1. *The state ω on $\mathrm{CAR}(\mathbb{D})$ is a Hadamard state if*

$$\mathrm{WF}(\mathbb{L}^\pm)' \subset \mathcal{N}^\pm \times \mathcal{N}^\pm.$$

We have the following version of Proposition 17.12.2.

Proposition 17.14.2. *Let $l^\pm_\Sigma =: \mathrm{i}\Gamma(n)c^\pm$, where $c^\pm$ are linear continuous from $C_0^\infty(\Sigma; \mathbb{S}^*_\Sigma)$ to $C^\infty(\Sigma; \mathbb{S}^*_\Sigma)$ and from $\mathcal{E}'(\Sigma; \mathbb{S}^*_\Sigma)$ to $\mathcal{D}'(\Sigma; \mathbb{S}^*_\Sigma)$. Assume that*

$$\mathrm{WF}(\mathbb{U}_\Sigma \circ c^\pm)' \subset \mathcal{N}^\pm \times (T^*\Sigma \setminus o) \ \text{ over } U \times \Sigma,$$

for some neighborhood U of Σ in M. Then ω is a Hadamard state.

17.15. Relationship between Dirac and Weyl Hadamard states

Finally, let us describe the relationship between Hadamard states for the Weyl and Dirac equations.

PROPOSITION 17.15.1. *Let $\omega_{\mathbb{D}}$ be a quasi-free Hadamard state for $\mathbb{D}$ with spacetime covariances $\mathbb{L}^{\pm}$. Then*

$$\Lambda^{\pm} = \begin{pmatrix} 0 & \mathbb{L}^{\pm}\beta \\ -\kappa\mathbb{L}^{\mp}\beta\kappa & 0 \end{pmatrix}$$

are the spacetime covariances of a quasi-free Hadamard state ω_D for $\not{D}$.

Proof. We check (17.32). Condition (i) is obvious. We have $(\mathbb{L}^{+}+\mathbb{L}^{-})\beta = \mathrm{i}\mathbb{G}\beta = \mathrm{i}G$ on $C_0^{\infty}(M;\mathcal{W}_{\mathrm{o}})$, hence $\kappa(\mathbb{L}^{+}+\mathbb{L}^{-})\beta\kappa = -\mathrm{i}\kappa G\kappa = -\mathrm{i}G$ on $C_0^{\infty}(M;\mathcal{W}_{\mathrm{e}})$, since $\kappa G = G\kappa$ and κ is anti-linear, which proves condition (iii). Condition (iv) is also immediate. To check the positivity condition (ii), we write using (17.13) and the fact that $\beta = \beta^{*}$:

$$\begin{aligned}(\psi|\beta\Lambda^{\pm}\psi) = &\quad (\psi_{\mathrm{o}}|\beta\mathbb{L}^{\pm}\beta\psi_{\mathrm{o}}) - (\psi_{\mathrm{e}}|\beta\kappa\mathbb{L}^{\mp}\beta\kappa\psi_{\mathrm{e}}) \\ = &\quad (\psi_{\mathrm{o}}|\beta\mathbb{L}^{\pm}\beta\psi_{\mathrm{o}}) + (\kappa\psi_{\mathrm{e}}|\beta\mathbb{L}^{\mp}\beta\kappa\psi_{\mathrm{e}}) \\ = &\quad (\psi_{\mathrm{o}}|\beta\mathbb{L}^{\pm}\beta\psi_{\mathrm{o}}) + (\beta\kappa\psi_{\mathrm{e}}|\mathbb{L}^{\mp}\beta\kappa\psi_{\mathrm{e}}) \geq 0,\end{aligned}$$

as needed. It remains to prove the Hadamard condition. The fact that $\mathrm{WF}(\mathbb{L}^{\pm}\beta)' \subset \mathcal{N}^{\pm}\times\mathcal{N}^{\pm}$ follows from the Hadamard property of $\omega_{\mathbb{D}}$. This implies that $\mathrm{WF}(\kappa L^{\pm}\beta\kappa) \subset \mathcal{N}^{\mp}\times\mathcal{N}^{\mp}$ since κ is anti-linear, and completes the proof that $\omega_{\not{D}}$ is Hadamard. □

The converse of Proposition 17.15.1 is much easier.

PROPOSITION 17.15.2. *Let $\Lambda^{\pm}$ be the spacetime covariances of a Hadamard state for $\not{D}$. Then setting $\Lambda^{\pm}_{\mathrm{o}} = \Lambda^{\pm}|_{C_0^{\infty}(M;\mathcal{W}_{\mathrm{o}})}$, the maps*

$$\mathbb{L}^{\pm} = \Lambda^{\pm}_{\mathrm{o}}\beta^{-1}$$

are the covariances of a Hadamard state for $\mathbb{D}$.

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General index

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