AN INTRODUCTION TO QUANTUM FIELD THEORY ON CURVED SPACE-TIMES

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1. Introduction

The purpose of these notes is to give an introduction to some recent aspects of Quantum Field Theory on curved space-times, emphasizing its relations with partial differential equations and microlocal analysis.

1.1. **Quantum Field Theory.** Quantum Field Theory arose from the need to unify Quantum Mechanics with special relativity. However trying to treat the two basic relativistic field equations, the *Klein-Gordon equation* :

$$\partial_t^2\phi(t,x)-\Delta_x\phi(t,x)+m^2\phi(t,x)=0,\ \ (t,x)\in\mathbb{R}^{1+d},$$

and the *Dirac equation* :

$$\gamma^0\partial_t\psi(t,x)+\gamma^i\partial_{x^i}\psi(t,x)-m\psi(t,x)=0\ (t,x)\in\mathbb{R}^{1+d},$$

(where the γ^i are the Dirac matrices) in a way parallel to the non-relativistic *Schroedinger equation* :

$$\partial_t\psi(t,x)-\frac{\mathrm{i}}{2m}\Delta_x\psi(t,x)+\mathrm{i}V(x)\psi(t,x)=0$$

leads to difficulties (see eg [BD]). For the Klein-Gordon equation, there exists a conserved scalar product :

$$\langle\phi_1|\phi_2\rangle=\mathrm{i}\int_{\mathbb{R}^d}\partial_t\overline{\phi}_1(t,x)\phi_2(t,x)-\overline{\phi}_1(t,x)\phi_2(t,x)dx$$

which is not positive definite, hence cannot lead to a probabilistic interpretation. However on has

$$\langle\phi|\mathrm{i}\partial_t\phi\rangle\geq 0,\ \ \text{(positivity of the energy)}.$$

For the Dirac equation the situation is the opposite : the conserved scalar product

$$\langle\psi_1|\psi_2\rangle=\int_{\mathbb{R}^d}\overline{\psi}_1(t,x)\cdot\psi_2(t,x)dx$$

is positive, but

$$\langle\psi|\mathrm{i}\partial_t\psi\rangle\text{ is indefinite.}$$

Hence it is possible to give a quantum mechanical interpretation of Dirac's equation, but the Hamiltonian will be unbounded below. This last issue was solved by Dirac, first by introducing the notion of the *Dirac sea*, then a few years later by interpreting negative energy states as wave functions for the recently discovered *positron.*

The reason behind these difficulties is that, although all these equations are partial differential equations, their nature is very different : the Klein-Gordon and Dirac equations are *classical* equations, while the Schroedinger equation is a *quantum* equation, obtained by quantizing the classical *Newton equation* :

$$\ddot{x}(t) = -\nabla_x V(x(t)), \; x \in \mathbb{R}^n.$$

or equivalently the Hamilton equations :

$$\begin{cases} \dot{x}(t) = \partial_\xi h(x(t), \xi(t)), \\ \dot{\xi}(t) = -\partial_x h(x(t), \xi(t)) \end{cases}$$

for the classical Hamiltonian :

$$h(x, \xi) = \frac{1}{2}\xi^2 + V(x).$$

Let us denote by $X = (x, \xi)$ the points in $T^*\mathbb{R}^n$ and introduce the coordinate functions

$$q : X \mapsto x, \; p : X \mapsto \xi.$$

If $\Phi(t) : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ is the flow of H_h and $q(t) := q \circ \Phi(t)$, $p(t) := p \circ \Phi(t)$ then :

$$\begin{aligned} \partial_t q(t) &= p(t), \\ \partial_t p(t) &= -\nabla V(q(t)), \end{aligned}$$

which is known as the *Liouville equation.* Note that

$$\{p_j(t), q_k(t)\} = \delta_{jk}, \; \{p_j(t), p_k(t)\} = \{q_j(t), q_k(t)\} = 0,$$

where $\{\cdot, \cdot\}$ is the Poisson bracket. To quantize the Liouville equation means to find a Hilbert space $\mathcal{H}$ and functions $\mathbb{R} \ni t \mapsto p(t), q(t)$ with values in selfadjoint operators on $\mathcal{H}$ such that

$$\begin{aligned} &[p_j(t), \mathrm{i}q_k(t)] = \delta_{jk}\mathbb{1}, \; [p_j(t), \mathrm{i}p_k(t)] = [q_j(t), \mathrm{i}q_k(t)] = 0, \\ &\partial_t q(t) = p(t), \\ &\partial_t p(t) = -\nabla V(q(t)). \end{aligned} \tag{1.1}$$

The equations in the first time are called the (fixed time) *canonical commutation relations.* The last two equations are called *Heisenberg* equations. The solution is as follows :

(1) Find operators p, q satisfying

$$[p_j, \mathrm{i}q_k] = \delta_{jk}\mathbb{1}, \; [p_j, \mathrm{i}p_k] = [q_j, \mathrm{i}q_k] = 0.$$

(2) Construct the following selfadjoint operator on $\mathcal{H}$

$$H = \frac{1}{2}p^2 + V(q).$$

Then

$$q(t) := \mathrm{e}^{\mathrm{i}tH} q \mathrm{e}^{-\mathrm{i}tH}, \; p(t) := \mathrm{e}^{\mathrm{i}tH} p \mathrm{e}^{-\mathrm{i}tH}$$

solve (1.1).

The *Stone-von Neumann theorem* says that there is no choice in step (1) : modulo some technical conditions and multiplicity one has only one choice, up to unitary equivalence :

$$\mathcal{H} = L^2(\mathbb{R}^n), \; q = x, \; p = \mathrm{i}^{-1}\nabla_x.$$

Then $H = -\frac{1}{2}\Delta + V(x)$ is the Schroedinger operator. step (2) is then a standard problem in the theory of selfadjoint operators.

The Klein-Gordon equation is also a Hamiltonian equation, however with a *infinite dimensional* phase space, which can be taken for example as $C_0^\infty(\mathbb{R}^d) \oplus C_0^\infty(\mathbb{R}^d)$. The classical Hamiltonian is then

$$h(\varphi, \pi) := \frac{1}{2}\int_{\mathbb{R}^d} \pi^2(x) + |\nabla_x \varphi(x)|^2 + m^2\varphi^2(x)dx,$$

for the linear case, or

$$h(\varphi, \pi) := \frac{1}{2}\int_{\mathbb{R}^d} \pi^2(x) + |\nabla_x \varphi(x)|^2 + m^2\varphi^2(x) + \varphi^n(x)dx,$$

for some non-linear version. Here the symbols $\varphi(x)$, $\pi(x)$ are (coordinate) functions, parametrized by a point $x \in \mathbb{R}^d$, on the space of smooth solutions of the Klein-Gordon equation, with compactly supported Cauchy data. If ϕ is such a solution then

$$\varphi(x)(\phi) := \phi(0, x), \ \pi(x)(\phi) := \partial_t\phi(0, x)$$

It is well-known that these are *symplectic coordinates*, i.e.

$$\{\varphi(x), \varphi(x')\} = \{\pi(x), \pi(x')\} = 0, \ \{\pi(x), \phi(x')\} = \delta(x, x'), \ \forall \ x, x' \in \mathbb{R}^d.$$

One would like to follow the same path and consider families of operators on a Hilbert space $\mathcal{H}$, $\varphi(x)$, $\pi(x)$, $x \in \mathbb{R}^d$ such that

$$[\pi(x), \mathrm{i}\varphi(x')] = \delta(x - x')\mathbb{1}, \ [\varphi(x), \mathrm{i}\varphi(x')] = [\pi(x), \mathrm{i}\pi(x')] = 0, \ \forall \ x, x' \in \mathbb{R}^d.$$

The fundamental difference with non-relativistic Quantum Mechanics is that, since the phase space is infinite dimensional, the Stone von Neumann theorem cannot be applied anymore : there exists an infinite number of inequivalent representations of commutation relations.

In other words, when one tries to quantize a classical field equation, the Hilbert space has to be constructed *together* with the quantum Hamiltonian : one cannot work on our familiar Hilbert space and then use tools from operator theory to construct the quantum Hamiltonian.

This is the reason why the rigorous construction of Quantum Field Theory models is so difficult, except for *non-interacting* theories. For interacting theories it has been achieved only in 2 and 3 spacetime dimensions, see the construction of the $P(\varphi)_2$ and φ_3^4 models, which were the landmark successes of *constructive field theory*. In 4 spacetime dimensions one has to rely instead on perturbative methods.

Another lesson learned from Quantum Field Theory (and also from Quantum Statistical Mechanics), is that Hilbert spaces do not play such a central role anymore. Instead one focuses on *algebras* and *states*.

Let us finish this discussion by recalling a well-known anecdote : at the Solvay conference in 1927, Dirac told Bohr that he was trying to find a relativistic quantum theory of the electron (i.e. the Dirac equation). Bohr replied that this problem had already been solved by Klein, who had found the Klein-Gordon equation. We know now that these two equations are of a different nature, the first describing fermionic fields, the second bosonic ones, and that they can be interpreted as quantum equations only via Quantum Field Theory.

1.2. **QFT on curved space-times.** Given the difficulties with the construction of interacting field theories on Minkowski space-time, one may wonder why one should consider quantum field theories on *curved space-times*, which have no reason to be simpler.

One reason comes from attempts to quantize gravitation, where one starts by linearizing Einstein equations around a curved background metric g. Another argument is that there are several interesting quantum effects appearing in presence of strong gravitational fields. The most famous one is the *Hawking effect*, which predicts that a black hole can emit quantum particles.

There are several new challenges one has to face when moving from flat Minkowski space-time to an arbitrary curved space-time.

On the computational side, one cannot rely anymore on the *Fourier transform* and related analyticity arguments, which are natural and useful on Minkowski space, since the Klein-Gordon equation has then constant coefficients.

On a more conceptual side, a curved space-time does not have the large group of isometries (the Poincaré group) of the Minkowski space. It follows that on a curved space-time there seems to be no natural notion of a *vacuum state*, which is defined on Minkowski space as the unique state which is invariant under space-time translations, and has an additional *positive energy condition.*

In the eigthies, physicists managed to define a class of states, the so-called *Hadamard states*, which were characterized by properties of their two-point functions, which had to have a specific asymptotic expansion near the diagonal, connected with the Hadamard parametrix construction for the Klein-Gordon equation on a curved space-time.

Later in 1995, in a seminal paper, Radzikowski reformulated the old Hadamard condition in terms of the *wave front set* of the two-point function. The wave front set of a distribution, introduced in 1970 by Hörmander, is one of the important notions of *microlocal analysis*, a theory which was precisely developed to extend Fourier analysis, in the study of general partial differential equations.

The introduction of tools from microlocal analysis had a great influence on the field, leading for example to the proof of renormalizability of scalar interacting field theories by Brunetti and Fredenhagen [BF].

The goal of these notes is to give an introduction to the modern notion of Hadamard states, for a mathematically oriented audience.

2. A quick introduction to Quantum Mechanics

This section is supposed to give a very quick introduction to the mathematical formalism of Quantum Mechanics, which is (or is expected to be) still relevant to Quantum Field Theory.

2.1. **Hilbert space approach.** In ordinary Quantum Mechanics, the description of a physical system starts with a Hilbert space $\mathcal{H}$, whose scalar product is denoted by $(u|v)$. The *states* of the system are described by unit vectors $\psi \in \mathcal{H}$ with $\|\psi\| = 1$.

The various physical quantities which can be measured (like position, momentum, energy, spin) are represented by *selfadjoint operators* on $\mathcal{H}$, i.e. (forgetting about important issues with unbounded operators), linear operators A on $\mathcal{H}$, assumed to be bounded for simplicity, such that $A = A^*$, (where A^* is the *adjoint* of A), called *observables.*

If $\psi \in \mathcal{H}$, $\|\psi\| = 1$ is a state vector, then the map :

$$A \mapsto \omega_\psi(A) = (\psi|A\psi)$$

computes the *expectation value* of A in the state ψ represent the average value of actual measurements of the physical quantity represented by A.

Rather quickly people were led to consider also *mixed states*, where the state of the system is only incompletely known. For example if ψ_i, $i \in \mathbb{N}$ is an orthonormal family and $0 \leq \rho_i \leq 1$ are real numbers with $\sum_{i=0}^{\infty} \rho_i = 1$, then we can consider the trace-class operator :

$$\rho = \sum_{i=0}^{\infty} \rho_i |\psi_i)(\psi_i|, \ \mathrm{Tr}\rho = 1,$$

called a *density matrix* and the map

$$A \mapsto \omega_\rho(A) := \mathrm{Tr}(\rho A)$$

is called a *mixed state*. Vector states are also called *pure states*.

2.2. **Algebraic approach.** The framework above is sufficient to cover all of non-relativistic Quantum Mechanics, i.e. in practice quantum systems consisting of a *finite* number of non-relativistic particles. However when one considers systems with an *infinite* number of particles, like in statistical mechanics, or quantum field theory, where the notion of particles is dubious, an algebraic framework is more relevant. It starts with the following observation about the space $B(\mathcal{H})$ of bounded operators on $\mathcal{H}$:

if we equip it with the operator norm, it is a Banach space, and a Banach algebra, i.e. an algebra with the property that $\|AB\| \leq \|A\|\|B\|$. It is also an involutive Banach algebra, i.e. the adjoint operation $A \mapsto A^*$ has the properties that

$$(AB)^* = B^* A^*, \ \|A^*\| = \|A\|.$$

Finally one can easily check that :

$$\|A^* A\| = \|A\|^2, \ A \in B(\mathcal{H}).$$

This last property has very important consequences, for example one can deduce from it the functional calculus and spectral theorem for selfadjoint operators.

An abstract algebra $\mathfrak{A}$ equipped with a norm and an involution with these properties, which is moreover complete is called a *C^* algebra*. The typical example of a C^* algebra is of course the algebra $B(\mathcal{H})$ of bounded operators on a Hilbert space.

If $\mathcal{H}$ is a Hilbert space, a $*-$homomorphism

$$\mathfrak{A} \ni A \mapsto \pi(A) \in B(\mathcal{H})$$

is callled a *representation* of $\mathfrak{A}$ in $\mathcal{H}$. An injective representation is called *faithful*.

The need for such change of point of view comes from the fact that a physical system, like a gas of electrons, can exist in many different physical realizations, for example at different temperatures. In other words it does not come equipped with a canonical Hilbert space.

Observables, like for example the electron density, have a meaning irrelevant of the realizations, and are described by selfadjoint elements in some C^* algebra $\mathfrak{A}$. However the various Hilbert spaces and the representations of the observables on them are very different from one temperature to another.

One can also describe the possible physical realizations of a system with the language of *states*. A *state* ω on $\mathfrak{A}$ is a linear map :

$$\omega : \mathfrak{A} \mapsto \mathbb{C}$$

such that

$$\omega(A^*A) \geq 0, \; A \in \mathfrak{A}.$$

Assuming that $\mathfrak{A}$ has a unit (which can always be assumed by adjoining one), one also requires that

$$\omega(\mathbb{1}) = 1.$$

The set of states on a C^* algebra is a convex set, its extremal points are called *pure states.* If $\mathfrak{A} \subset B(\mathcal{H})$ and ψ is a unit vector, or if ρ is a density matrix, then

$$\omega_\psi(A) := (\psi|A\psi), \; \omega_\rho(A) := \mathrm{Tr}(\rho A)$$

are states on $\mathfrak{A}$. If $\mathfrak{A} = B(\mathcal{H})$, then ω_ψ is a pure state. It is important to be aware of the fact that if $\mathfrak{A}$ is only a C^* subalgebra of $B(\mathcal{H})$, then ω_ψ may *not* be a pure state on $\mathfrak{A}$.

2.3. **The GNS construction.** After being told that one should use C^* algebras and states, one can wonder where the Hilbert spaces have gone. Actually given a C^* algebra $\mathfrak{A}$ and a state ω on it, it is quite easy to construct a canonical Hilbert space and a representation of $\mathfrak{A}$ on it, as proved by Gelfand, Naimark and Segal. There exist a triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, unique up to unitary equivalence, where $\mathcal{H}_\omega$ is a Hilbert space, $\pi_\omega : \mathfrak{A} \mapsto B(\mathcal{H}_\omega)$ is a faithful representation, $\Omega_\omega \in \mathcal{H}_\omega$ is a unit vector such that :

$$\omega(A) = (\Omega_\omega|\pi_\omega(A)\Omega_\omega), \; A \in \mathfrak{A},$$

and $\{\pi_\omega(A)\Omega_\omega \; : \; A \in \mathfrak{A}\}$ is dense in $\mathcal{H}_\omega$.

3. Notation

In this section we collect some notation that will be used in these notes. If $\mathcal{X}$ is a real or complex vector space we denote by $\mathcal{X}^\#$ its dual. Bilinear forms on $\mathcal{X}$ are identified with elements of $L(\mathcal{X}, \mathcal{X}^\#)$, which leads to the notation $x_1 b x_2$ for $b \in L(\mathcal{X}, \mathcal{X}^\#)$, $x_1, x_2 \in \mathcal{X}$. The space of symmetric (resp. anti-symmetric) bilinear forms on $\mathcal{X}$ is denoted by $L_{\rm s}(\mathcal{X}, \mathcal{X}^\#)$ (resp. $L_{\rm a}(\mathcal{X}, \mathcal{X}^\#)$).

If $\sigma \in L_{\rm s}(\mathcal{X}, \mathcal{X}^\#)$ is non-degenerate, we denote by $O(\mathcal{X}, \sigma)$ the linear (pseudo-)orthogonal group on $\mathcal{X}$. Similarly if $\sigma \in L_{\rm a}(\mathcal{X}, \mathcal{X}^\#)$ is non-degenerate, i.e. $(\mathcal{X}, \sigma)$ is a symplectic space, we denote by $Sp(\mathcal{X}, \sigma)$ the linear symplectic group on $\mathcal{X}$.

If $\mathcal{Y}$ is a complex vector space, we denote by $\mathcal{Y}_\mathbb{R}$ its *realification*, i.e. $\mathcal{Y}$ considered as a real vector space. We denote by $\overline{\mathcal{Y}}$ a *conjugate vector space* to $\mathcal{Y}$, i.e. a complex vector space $\overline{\mathcal{Y}}$ with an anti-linear isomorphism $\mathcal{Y} \ni y \mapsto \overline{y} \in \overline{\mathcal{Y}}$. The *canonical conjugate vector space* to $\mathcal{Y}$ is simply the real vector space $\mathcal{Y}_\mathbb{R}$ equipped with the complex structure $-\mathrm{i}$, if i is the complex structure of $\mathcal{Y}$. In this case the map $y \to \overline{y}$ is chosen as the identity. If $a \in L(\mathcal{Y}_1, \mathcal{Y}_2)$, we denote by $\overline{a} \in L(\overline{\mathcal{Y}}_1, \overline{\mathcal{Y}}_2)$ the linear map defined by :

$$\overline{a}\overline{y}_1 := \overline{ay_1}, \; \overline{y}_1 \in \overline{\mathcal{Y}}_1. \tag{3.1}$$

We denote by $\mathcal{Y}^*$ the *anti-dual* of $\mathcal{Y}$, i.e. the space of anti-linear forms on $\mathcal{Y}$. Clearly $\mathcal{Y}^*$ can be identified with $\overline{\mathcal{Y}^\#} \sim \overline{\mathcal{Y}}^\#$.

Sesquilinear forms on $\mathcal{Y}$ are identified with elements of $L(\mathcal{Y}, \mathcal{Y}^*)$, and we use the notation $(y_1|by_2)$ or $\overline{y_1}\cdot by_2$ for $b \in L(\mathcal{Y}, \mathcal{Y}^*)$, $y_1, y_2 \in \mathcal{Y}$.

The space of hermitian (resp. anti-hermitian) sesquilinear forms on $\mathcal{Y}$ is denoted by $L_{\rm s}(\mathcal{Y}, \mathcal{Y}^*)$ (resp. $L_{\rm a}(\mathcal{Y}, \mathcal{Y}^*)$).

If $q \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$ is non-degenerate, i.e. $(\mathcal{Y}, q)$ is a pseudo-unitary space, we denote by $U(\mathcal{Y}, q)$ the linear pseudo-unitary group on $\mathcal{Y}$.

If b is a bilinear form on the real vector space $\mathcal{X}$, its canonical sesquilinear extension to $\mathbb{C}\mathcal{X}$ is by definition the sesquilinear form $b_{\mathbb{C}}$ on $\mathbb{C}\mathcal{X}$ given by

$$(w_1|b_{\mathbb{C}}w_2) := x_1\cdot bx_2 + y_1\cdot by_2 + {\rm i}x_1\cdot by_2 - {\rm i}y_1\cdot bx_2, \quad w_i = x_i + {\rm i}y_i$$

for $x_i, y_i \in \mathcal{X}$, $i = 1, 2$. This extension maps (anti-)symmetric forms on $\mathcal{X}$ onto (anti-)hermitian forms on $\mathbb{C}\mathcal{X}$.

Conversely if $\mathcal{Y}$ is a complex vector space and $\mathcal{Y}_{\mathbb{R}}$ is its realification, i.e. $\mathcal{Y}$ considered as a real vector space, then for $b \in L_{\rm h/a}(\mathcal{Y}, \mathcal{Y}^*)$ the form ${\rm Re}b$ belongs to $L_{\rm s/a}(\mathcal{Y}_{\mathbb{R}}, \mathcal{Y}_{\mathbb{R}}^\#)$.

4. CCR and CAR algebras

4.1. **Introduction.** It is useful to discuss the CCR and CAR without making reference to a Fock space. There are some mathematical subtleties with CCR algebras, coming from the fact that the field operators are 'unbounded'. These subtleties can mostly be ignored for our purposes.

4.2. **Algebras generated by symbols and relations.** In physics many algebras are defined by specifying a set of generators and the relations they satisfy. This is completely sufficient to do computations, but mathematicians may feel uncomfortable with such an approach. However it is easy (and actually rather useless) to give a rigorous definition.

Assume that $\mathcal{A}$ is a set. We denote by $c_{\rm c}(\mathcal{A}, \mathbb{K})$ the vector space of functions $\mathcal{A} \to \mathbb{K}$ with finite support (usually $\mathbb{K} = \mathbb{C}$). If for $A \in \mathcal{A}$, we denote the indicator function $\mathbb{1}_{\{A\}}$ simply by A, we see that any element of $c_{\rm c}(\mathcal{A}, \mathbb{K})$ can be written as $\sum_{A\in\mathcal{B}} \lambda_A A$, $\mathcal{B} \subset \mathcal{A}$ finite, $\lambda_A \in \mathbb{K}$.

Then $c_{\rm c}(\mathcal{A}, \mathbb{K})$ can be seen as the vector space of finite linear combinations of elements of $\mathcal{A}$. We set

$$\mathfrak{A}(\mathcal{A}, \mathbb{1}) := \overset{\rm al}{\otimes} c_{\rm c}(\mathcal{A}, \mathbb{K}),$$

called the *universal unital algebra over* $\mathbb{K}$ *with generators* $\mathcal{A}$. Usually one write $A_1 \cdots A_n$ instead of $A_1 \otimes \cdots \otimes A_n$ for $A_i \in \mathcal{A}$.

Let us denote by $\overline{\mathcal{A}}$ another copy of $\mathcal{A}$. We denote by $\overline{a}$ the element $a \in \overline{\mathcal{A}}$. We set then $*a := \overline{a}$, $*\overline{a} := a$ and extend $*$ to $\mathfrak{A}(\mathcal{A} \sqcup \overline{\mathcal{A}}, \mathbb{1})$ by setting

$$(b_1 b_2 \cdots b_n)^* = b_n^* \cdots b_2^* b_1^*, \quad b_i \in \mathcal{A} \sqcup \overline{\mathcal{A}}, \ \mathbb{1} = \mathbb{1}^*.$$

The algebra $\mathfrak{A}(\mathcal{A} \sqcup \overline{\mathcal{A}}, \mathbb{1})$ equipped with the involution $*$ is called the *universal unital* $^*-$*algebra over* $\mathbb{K}$ *with generators* $\mathcal{A}$.

Let now $\mathfrak{R} \subset \mathfrak{A}(\mathcal{A}, \mathbb{1})$ (the set of 'relations'). We denote by $\mathfrak{I}(\mathfrak{R})$ the ideal of $\mathfrak{A}(\mathcal{A}, \mathbb{K})$ generated by $\mathfrak{R}$. Then the quotient

$$\mathfrak{A}(\mathcal{A}, \mathbb{1})/\mathfrak{I}(\mathfrak{R})$$

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

Similarly if $\mathfrak{R} \subset \mathfrak{A}(\mathcal{A} \cup \overline{\mathcal{A}}, \mathbb{1})$ is $*$-invariant, then $\mathfrak{A}(\mathcal{A} \sqcup \overline{\mathcal{A}}, \mathbb{1})/\mathfrak{I}(\mathfrak{R})$ is called the *unital* $*$*-algebra with generators* $\mathcal{A} \sqcup \overline{\mathcal{A}}$ *and relations* $R = 0, \quad R \in \mathfrak{R}$.

4.3. **Polynomial CCR algebra.** We fix a (real) presymplectic space $(\mathcal{X}, \sigma)$, i.e. $\sigma \in L_{\rm a}(\mathcal{X}, \mathcal{X}^{\#})$ is not supposed to be injective.

Definition 4.1. *The* polynomial CCR $*$-algebra over $\mathcal{X}$*, denoted by* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$*, is defined to be the unital complex* $*$*-algebra generated by elements* $\phi(x)$*,* $x \in \mathcal{X}$*, with relations*

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

4.4. **Weyl CCR algebra.** One problem with $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$ is that (unless $\sigma = 0$) its elements cannot be faithfully represented as bounded operators on a Hilbert space. To cure this problem one has to work with Weyl operators, which lead to the Weyl CCR $*-$algebra.

Definition 4.2. *The* algebraic Weyl CCR algebra over $\mathcal{X}$ *denoted by* $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ *is the* $*$*-algebra generated by the elements* $W(x)$*,* $x \in \mathcal{X}$*, with relations*

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

It is possible to equip $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ with a unique C^*-norm. Its completion for this norm is called the *Weyl CCR algebra over* $\mathcal{X}$ and still denoted by $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$. We will mostly work with $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X}, \sigma)$, which will simply be denoted by $\mathrm{CCR}(\mathcal{X}, \sigma)$. Of course the formal relation between the two approaches is

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

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

4.5. **Charged symplectic spaces.**

Definition 4.3. *A complex vector space* $\mathcal{Y}$ *equipped with a a non-degenerate anti-hermitian sesquilinear form* σ *is called a* charged symplectic space*. We set*

$$
q := \mathrm{i}\sigma \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*),
$$

which is called the charge*.*

4.6. **Kähler spaces.** Let $(\mathcal{Y}, \sigma)$ be a charged symplectic space. Its complex structure will be denoted by $\mathrm{j} \in L(\mathcal{Y}_{\mathbb{R}})$ (to distinguish it from the complex number $\mathrm{i} \in \mathbb{C}$). Note that $(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ is a real symplectic space with $\mathrm{j} \in Sp(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ and $\mathrm{j}^2 = -\mathbb{1}$. We have :

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

The converse construction is as follows : A real (pre-)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 :

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

and check that q is sesquilinear hermitian on $\mathcal{Y}$ equipped with the complex structure j. One can consider the CCR algebra $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$, with selfadjoint generators $\phi(y)$ and relations :

$$[\phi(y_1), \phi(y_2)] = \mathrm{i} y_1 \cdot \mathrm{Re}\sigma y_2 \mathbb{1}.$$

One can instead generate $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ by the *charged fields* :

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

The map $\mathcal{Y} \ni y \mapsto \psi^*(y)$ (resp. $\mathcal{Y} \ni y \mapsto \psi(y)$) is $\mathbb{C}-$linear (resp. $\mathbb{C}-$anti-linear). The commutation relations take the form :

$$\begin{aligned}
&[\psi(y_1), \psi(y_2)] = [\psi^*(y_1), \psi^*(y_2)] = 0, \\
&[\psi(y_1), \psi^*(y_2)] = \overline{y}_1 \cdot q y_2 \mathbb{1}, \ y_1, y_2 \in \mathcal{Y}.
\end{aligned}$$

Note the similarity with the CCR expressed in terms of creation/annihilation operators, the difference being the fact that q is not necessarily positive. In this context, it is natural to denote $\mathrm{CCR}(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\sigma)$ by $\mathrm{CCR}(\mathcal{Y}, \sigma)$.

4.7. **CAR algebra.** We fix an Euclidean space $(\mathcal{X}, \nu)$ (possibly infinite dimensional).

Definition 4.4. *The* algebraic CAR algebra over $\mathcal{X}$, *denoted* $\mathrm{CAR}^{\mathrm{alg}}(\mathcal{X}, \nu)$, *is the complex unital $*$-algebra generated by elements $\phi(x)$, $x \in \mathcal{X}$, with relations*

$$\begin{aligned}
&\phi(\lambda x) = \lambda \phi(x), \ \lambda \in \mathbb{R}, \qquad \phi(x_1 + x_2) = \phi(x_1) + \phi(x_2), \\
&\phi^*(x) = \phi(x), \qquad \phi(x_1)\phi(x_2) + \phi(x_2)\phi(x_1) = 2 x_1 \cdot \nu x_2 \mathbb{1}.
\end{aligned}$$

Again $\mathrm{CAR}^{\mathrm{alg}}(\mathcal{X}, \nu)$ has a unique C^*-norm, and its completion is denoted by $\mathrm{CAR}(\mathcal{X}, \nu)$.

4.8. **Kähler spaces.** Let now $(\mathcal{Y}, \nu)$ be a hermitian space, denoting again its complex structure by j. Then $(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\nu)$ is an euclidean space, with $\mathrm{j} \in U(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\nu)$. We have :

$$\overline{y}_1 \cdot \nu y_2 = y_1 \cdot \mathrm{Re}\nu y_2 - \mathrm{i} y_1 \cdot \mathrm{Rej} y_2, \ y_1, y_2 \in \mathcal{Y}.$$

Denoting by $\phi(y)$ the selfadjoint fields which generate $\mathrm{CAR}(\mathcal{Y}_{\mathbb{R}}, \mathrm{Re}\nu)$, we can introduce the charged fields :

$$\psi(y) := \phi(y) + \mathrm{i}\phi(\mathrm{j}y), \ \psi^*(y) := \phi(y) - \mathrm{i}\phi(\mathrm{j}y), \ y \in \mathcal{Y}.$$

Again the map $\mathcal{Y} \ni y \mapsto \psi^*(y)$ (resp. $\mathcal{Y} \ni y \mapsto \psi(y)$) is $\mathbb{C}-$linear (resp. $\mathbb{C}-$anti-linear). The anti-commutation relations take the form :

$$\begin{aligned}
&[\psi(y_1), \psi(y_2)]_+ = [\psi^*(y_1), \psi^*(y_2)]_+ = 0, \\
&[\psi(y_1), \psi^*(y_2)]_+ = 2\overline{y}_1 \cdot \nu y_2 \mathbb{1}, \ y_1, y_2 \in \mathcal{Y}.
\end{aligned}$$

5. States on CCR/CAR algebras

5.1. **Introduction.** Let $\mathfrak{A}$ be a unital $*-$algebra. A *state* on $\mathfrak{A}$ is a linear map $\omega : \mathfrak{A} \to \mathbb{K}$ such that

$$\omega(A^*A) \geq 0, \ \forall A \in \mathfrak{A}, \ \omega(\mathbb{1}) = 1.$$

Elements of the form A^*A are called *positive.*

Let $\mathcal{X}$ be either a presymplectic or euclidean space and let ω be a state on $\mathrm{CCR}(\mathcal{X}, \sigma)$ or $\mathrm{CAR}(\mathcal{X}, \nu)$. One can associate to ω a bilinear form on $\mathcal{X}$ called the $2-$*point function* :

$$\mathcal{X} \times \mathcal{X} \ni (x_1, x_2) \mapsto \omega(\phi(x_1)\phi(x_2)).$$

Of course to completely specify the state ω one also needs to know the $n-$*point functions* :

$$\mathcal{X}^n \ni (x_1, \dots x_n) \mapsto \omega(\phi(x_1) \dots \phi(x_n)).$$

A particularly useful class of states are the *quasi-free* states, which are defined by the fact that all $n-$point functions are determined by the $2-$point function.

5.2. **Bosonic quasi-free states.** Let $(\mathcal{X}, \sigma)$ a presymplectic space and ω a state on $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$. The function :

$$\mathcal{X} \ni x \mapsto \omega(W(x)) =: G(x)$$

is called the *characteristic function* of the state ω, and is a non-commutative version of the Fourier transform of a probability measure.

There is also a non-commutative version of Bochner's theorem (the theorem which characterizes these Fourier transforms) :

Proposition 5.1. *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 $n \in \mathbb{N}$, $x_i \in \mathcal{X}$ 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. $\Rightarrow$: for $x_1, \dots, x_n \in \mathcal{X}$, $\lambda_1, \dots, \lambda_n \in \mathbb{C}$ set

$$A := \sum_{j=1}^{n} \lambda_j W(x_j) \in \mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma).$$

Such A are dense in $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$. One computes A^*A using the CCR and obtains that :

$$A^*A = \sum_{j,k=1}^{n} \overline{\lambda}_j \lambda_k W(x_j - x_k)\mathrm{e}^{\frac{\mathrm{i}}{2}x_j \cdot \sigma x_k},$$

from which $\Rightarrow$ follows.

$\Leftarrow$: one uses exactly the same argument, defining ω using G, the above formula shows that ω is positive. $\Box$

Definition 5.2. (1) *A state ω on* $\mathrm{CCR}^{\mathrm{Weyl}}(\mathcal{X}, \sigma)$ *is a* quasi-free state *if there exists $\eta \in L_{\mathrm{s}}(\mathcal{X}, \mathcal{X}^{\#})$ (a symmetric form on $\mathcal{X}$) such that*

$$\omega\big(W(x)\big) = \mathrm{e}^{-\frac{1}{2}x \cdot \eta x}, \quad x \in \mathcal{X}. \tag{5.1}$$

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

Quasi-free states should be considered as non-commutative versions of *Gaussian measures.* To explain this remark, consider the Gaussian measure on $\mathbb{R}^d$ with covariance η

$$\mathrm{d}\mu_\eta := (2\pi)^{d/2} \det \eta^- \frac{1}{2} \mathrm{e}^{-\frac{1}{2} y \cdot \eta^{-1} y} dy.$$

We have :

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

Note also that if $x_i \in \mathbb{R}^d$, then

$$\begin{array}{l} \int \prod_1^{2n+1} x_i \cdot y \mathrm{d}\mu_\eta(y) = 0, \\ \int \prod_1^{2n} x_i \cdot y \mathrm{d}\mu_\eta(y) = \sum_{\sigma \in \mathrm{Pair}_{2n}} \prod_{j=1}^n x_{\sigma(2j-1)} \cdot \eta x_{\sigma(2j)}, \end{array}$$

which should be compared with Def. 5.4 below.

Proposition 5.3. *Let* $\eta \in L_{\mathrm{s}}(\mathcal{X}, \mathcal{X}^\#)$. *Then the following are equivalent :*

(1) $\mathcal{X} \ni x \mapsto \mathrm{e}^{-\frac{1}{2} x \cdot \eta x}$ *is a characteristic function and hence there exists a quasi-free state satisfying (5.1).*

(2) $\eta_{\mathbb{C}} + \frac{\mathrm{i}}{2} \sigma_{\mathbb{C}} \geq 0$ *on* $\mathbb{C}\mathcal{X}$, *where* $\eta_{\mathbb{C}}, \sigma_{\mathbb{C}} \in L\big(\mathbb{C}\mathcal{X}, (\mathbb{C}\mathcal{X})^*\big)$ *are the canonical sesquilinear extensions of* η, σ.

(3) $|x_1 \cdot \sigma x_2| \leq 2(x_1 \cdot \eta x_1)^{\frac{1}{2}} (x_2 \cdot \eta x_2)^{\frac{1}{2}}, \ \ x_1, x_2 \in \mathcal{X}$.

Proof. The proof of (1) $\Rightarrow$ (2) is easy, by considering complex fields $\phi(w) = \phi(x_1) + \mathrm{i}\phi(x_2)$, $w = x_1 + \mathrm{i}x_2$ and noting that the positivity of ω implies that $\omega(\phi^*(w)\phi(w)) \geq 0$, for any $w \in \mathbb{C}\mathcal{X}$.

The proof of (2) $\Rightarrow$ (1) is more involved : let us fix $x_1, \dots, x_n \in \mathcal{X}$ and set

$$b_{jk} = x_j \cdot \eta x_k + \frac{\mathrm{i}}{2} x_j \cdot \sigma x_k.$$

Then, for $\lambda_1, \dots, \lambda_n \in \mathbb{C}$,

$$\sum_{1 \leq j,k \leq n} \overline{\lambda_j} b_{jk} \lambda_k = \overline{w} \cdot \eta_{\mathbb{C}} w + \tfrac{\mathrm{i}}{2} \overline{w} \cdot \omega_{\mathbb{C}} w, \quad w = \sum_{j=1}^n \lambda_j x_j \in \mathbb{C}\mathcal{X}.$$

By (2), the matrix $[b_{jk}]$ is positive. One has then to use an easy lemma, saying that the pointwise product of two positive matrices is positive. From this it follows also that $[\mathrm{e}^{b_{jk}}]$ is positive, and hence the matrix $[\mathrm{e}^{-\frac{1}{2} x_j \cdot \eta x_j} \mathrm{e}^{b_{jk}} \mathrm{e}^{-\frac{1}{2} x_k \cdot \eta x_k}]$ is positive. Hence :

$$\begin{array}{rl} & \sum_{j,k=1}^n \mathrm{e}^{-\frac{1}{2}(x_k - x_j) \cdot \eta (x_k - x_j)} \mathrm{e}^{\frac{\mathrm{i}}{2} x_j \cdot \omega x_k} \overline{\lambda}_j \lambda_k \\ = & \sum_{j,k=1}^n \mathrm{e}^{-\frac{1}{2} x_j \cdot \eta x_j} \mathrm{e}^{b_{jk}} \mathrm{e}^{-\frac{1}{2} x_j \cdot \eta x_j} \overline{\lambda}_j \lambda_k \\ = & \sum_{j,k=1}^n G(x_j - x_k) \mathrm{e}^{\frac{\mathrm{i}}{2} x_j \cdot \sigma x_k} \geq 0, \end{array}$$

for $G(x) = \mathrm{e}^{-\frac{1}{2} x \cdot \eta x}$. By Prop. 5.1, this means that G is a characteristic function. The proof of (2) $\Leftrightarrow$ (3) is an exercise in linear algebra. $\Box$

It is easy to deduce from ω the corresponding state acting on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$, by setting :

$$\begin{array}{rl} & \omega(\phi(x_1)\cdots\phi(x_n)) \\ := & \frac{\mathrm{d}}{dt_1}\cdots\frac{\mathrm{d}}{\mathrm{d}t_n}\omega(W(t_1x_1+\cdots+t_nx_n))_{|t_1=\cdots t_n=0}. \end{array}$$

In particular

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

The corresponding definition of a quasi-free state on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ is as follows :

Definition 5.4. *A state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ is* quasi-free *if*

$$\begin{array}{rcl} \omega\big(\phi(x_1)\cdots\phi(x_{2m-1})\big) & = & 0, \\ \omega\big(\phi(x_1)\cdots\phi(x_{2m})\big) & = & \sum_{\sigma\in\mathrm{Pair}_{2m}}\prod_{j=1}^{m}\omega\big(\phi(x_{\sigma(2j-1)})\phi(x_{\sigma(2j)})\big). \end{array}$$

We recall that Pair_{2m} is 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 partition $\sigma\in S_{2m}$ such that $\sigma(2k-1)=i_k$, $\sigma(2k)=j_k$.

5.3. **Gauge-invariant quasi-free states.** Let us now assume that $(\mathcal{X},\sigma,\mathrm{j})$ is a pseudo-Kähler space, i.e. that there exists an anti-involution $\mathrm{j}\in Sp(\mathcal{X},\sigma)$. Note that we have

$$\mathrm{e}^{\mathrm{j}\theta} = \cos\theta + \mathrm{j}\sin\theta,\ \ \theta\in\mathbb{R},$$

and the map :

$$[0,2\pi]\ni\theta\mapsto\mathrm{e}^{\mathrm{j}\theta}\in Sp(\mathcal{X},\sigma)$$

is a $1-$parameter group called the group of *(global) gauge transformations.*

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

$$\omega(W(x)) = \omega(W(\mathrm{e}^{\mathrm{j}\theta}x)),\ \ x\in\mathcal{X},\theta\in\mathbb{R}.$$

We can of course let ω act on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$. It is much more convenient then to use the *charged fields* $\psi^{(*)}(x)$ as generators of $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$. We have then :

Proposition 5.5. *A state ω on $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{X},\sigma)$ is gauge invariant quasi-free iff :*

$$\begin{array}{l} \omega\left(\Pi_1^n\psi^*(y_i)\Pi_1^p\psi(x_i)\right) = 0, \textit{if } n\neq p \\ \omega\left(\Pi_1^n\psi^*(y_i)\Pi_1^n\psi(x_i)\right) = \sum_{\sigma\in S_n}\prod_{i=1}^{n}\omega(\psi^*(y_i)\psi(x_{\sigma(i)})). \end{array}$$

It follows that a gauge invariant quasi-free state ω is uniquely determined by the sesquilinear form

$$\omega(\psi(y_1)\psi^*(y_2)) =: \overline{y}_1\cdot\lambda_+y_2.$$

Clearly $\lambda_+\in L_{\mathrm{h}}(\mathcal{Y},\mathcal{Y}^*)$. Let :

$$\omega(\psi^*(y_2)\psi(y_1)) =: \overline{y}_1\cdot\lambda_-y_2,$$

with $\lambda_- \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$. From the commutation relations we have of course :

$$\lambda_+ - \lambda_- = q,$$

so λ_- is determined by λ_+, but nevertheless it is convenient to work with the pair $(\lambda)_\pm$ and to call $\lambda_\pm$ the *complex covariances* of ω.

The link between the real and complex covariances is as follows :

Lemma 5.6. *We have :*

$$\eta = {\rm Re}(\lambda_\pm \mp \frac{1}{2}q),\ \ \hat{\eta} = \lambda_\pm \mp \frac{1}{2}q,$$

where $\hat{\eta} \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$ *is given by :*

$$\overline{y}_1 \hat{\eta} y_2 := y_1 \cdot \eta y_2 - {\rm i} y_1 \cdot \eta {\rm j} y_2.$$

Note that the fact that $\hat{\eta}$ is sesquilinear follows from the gauge-invariance of ω. From the above lemma one easily gets the following characterization of complex covariances.

Proposition 5.7. *Let* $\lambda_\pm \in L_{\rm h}(\mathcal{Y}, \mathcal{Y}^*)$. *Then the following are equivalent :*

(1) $\lambda_\pm$ *are the covariances of a gauge-invariant quasi-free state on* ${\rm CCR}^{\rm pol}(\mathcal{Y}, q)$*,*
(2) $\lambda_\pm \geq 0$ *and* $\lambda_+ - \lambda_- = q$.

Proof. Since ω is gauge-invariant we have

$$ {\rm j} \in O(\mathcal{Y}_\mathbb{R}, \eta) \cap Sp(\mathcal{Y}_\mathbb{R}, {\rm Re}\sigma) = O(\mathcal{Y}_\mathbb{R}, \eta) \cap O(\mathcal{Y}_\mathbb{R}, {\rm Re}q).$$

From this fact and Lemma 5.6 we deduce that $\eta \geq 0 \Leftrightarrow \lambda_+ \geq \frac{1}{2}q$, and that the second condition in Prop. 5.3 (with σ replaced by ${\rm Re}\sigma$) is equivalent to

$$\pm q \leq 2\lambda_+ - q \ \Leftrightarrow\ \lambda_\pm \geq 0.$$

This completes the proof of the proposition. □

5.4. **Complexifying bosonic quasi-free states.** If $(\mathcal{X}, \sigma)$ is real symplectic, we can form $(\mathbb{C}\mathcal{X}, \sigma_\mathbb{C})$ which is charged symplectic. As real symplectic space it equals $(\mathcal{X}, \sigma) \oplus (\mathcal{X}, \sigma)$. If ω is a quasi-free state on $(\mathcal{X}, \sigma)$ with real covariance η, we form a state $\omega_\mathbb{C}$ on $((\mathbb{C}\mathcal{X})_\mathbb{R}, {\rm Re}\sigma_\mathbb{C})$, with covariance ${\rm Re}\eta_\mathbb{C}$, which is by definition gauge invariant. Hence, possibly after complexification, we can always reduce ourselves to gauge invariant quasi-free states.

5.5. **Pure quasi-free states.** In this subsection we discuss *pure* quasi-free states, which turn out to be precisely *vacuum states.* To start the discussion, let us recall that from Prop. 5.3 (3) one has

$$|x_1 \cdot \sigma x_2| \leq 2(x_1 \cdot \eta x_1)^{\frac{1}{2}}(x_2 \cdot \eta x_2)^{\frac{1}{2}},\ \ x_1, x_2 \in \mathcal{X}. \tag{5.2}$$

We can complete the real vector space $\mathcal{X}$ w.r.t. the (semi-definite) symmetric form η, after taking the quotient by the vectors of zero norm as usual. Note that from (5.2) σ passes to quotient and to completion.

Denoting once again $(\mathcal{X}/{\rm Ker}\eta)^{\rm cpl}$ by $\mathcal{X}$, we end up with the following situation : $(\mathcal{X}, \eta)$ is a real Hilbert space, σ is a bounded, anti-symmetric form on $\mathcal{X}$. However σ may very well not be non-degenerate anymore, i.e. $(\mathcal{X}, \sigma)$ may just be pre-symplectic. One can show that if σ is degenerate, then the state on $\mathrm{CCR}(\mathcal{X},\sigma)$ with covariance η is not pure. In the sequel we hence assume that σ is non-degenerate on $\mathcal{X}$. One can then prove the following theorem. The proof uses some more advanced tools, like the Araki-Woods representation and its properties.

Theorem 5.8. *The state ω of covariance η is pure iff the pair $(2\eta,\sigma)$ is Kähler, that is there exists $\mathrm{j}\in Sp(\mathcal{X},\sigma)$ such that $\mathrm{j}^2=\mathbb{1}$ and $2\eta=\sigma\mathrm{j}$.*

The link with Fock spaces and vacuum states is now as follows : if one equips $\mathcal{X}$ with the complex structure j and the scalar product :

$$(x_1|x_2) := x_1\cdot 2\eta x_2 + \mathrm{i}x_1\cdot\eta\mathrm{j}x_2,$$

then $\mathcal{Z} := (\mathcal{X},(\cdot|\cdot))$ is a complex Hilbert space. One can build the bosonic Fock space $\Gamma_{\mathrm{s}}(\mathcal{Z})$ and the Fock representation $\mathcal{X}\ni x\mapsto \mathrm{e}^{\mathrm{i}\phi(x)}\in U(\Gamma_{\mathrm{s}}(\mathcal{Z}))$. This representation is precisely the GNS representation of the state ω, with GNS vector Ω_ω equal to the Fock vacuum.

For reference let us state the version of Thm. 5.8 using charged fields.

Theorem 5.9. *Let $\lambda_\pm\in L_{\mathrm{h}}(\mathcal{Y},\mathcal{Y}^*)$. Then the following are equivalent :*

(1) *$\lambda_\pm$ are the covariances of a* pure *gauge-invariant quasi-free state on* $\mathrm{CCR}^{\mathrm{pol}}(\mathcal{Y},\sigma)$,

(2) *there exists an involution $\kappa\in U(\mathcal{Y},q)$ such that $q\kappa\geq 0$ and $\lambda_\pm=\frac{1}{2}q(\kappa\pm\mathbb{1})$.*

(3) *$\lambda_\pm\geq\pm\frac{1}{2}q$, $\lambda_\pm q^{-1}\lambda_\pm=\pm\lambda_\pm$, $\lambda_+-\lambda_-=q$.*

Thm. 5.9 can be easily deduced from Thm. 5.8.

5.6. **Fermionic quasi-free states.** We consider now an Euclidean space $(\mathcal{X},\nu)$. Without loss of generality we can assume that $\mathcal{X}$ is complete, i.e. $(\mathcal{X},\nu)$ is a real Hilbert space. We consider the CAR algebra $\mathrm{CAR}(\mathcal{X},\nu)$, with the selfadjoint fermionic fields $\phi(x)$ as generators.

Definition 5.10. (1) *a state ω on $\mathrm{CAR}^{C^*}(\mathcal{X},\nu)$ is called* quasi-free *if*

$$\begin{aligned}\omega\big(\phi(x_1)\cdots\phi(x_{2m-1})\big) &= 0,\\ \omega\big(\phi(x_1)\cdots\phi(x_{2m})\big) &= \sum_{\sigma\in\mathrm{Pair}_{2m}}\mathrm{sgn}(\sigma)\prod_{j=1}^{m}\omega\big(\phi(x_{\sigma(2j-1)})\phi(x_{\sigma(2j)})\big),\end{aligned}$$

for all $x_1,x_2,\dots\in\mathcal{X}$, $m\in\mathbb{N}$.

(2) *the anti-symmetric form $\beta\in L_{\mathrm{a}}(\mathcal{X},\mathcal{X}^\#)$ defined by :*

$$x_1\cdot\beta x_2 := \mathrm{i}^{-1}\omega([\phi(x_1),\phi(x_2)])$$

is called the covariance *of the quasi-free state ω.*

From the CAR it follows that

$$\omega\big(\phi(x_1)\phi(x_2)\big) = x_1\cdot\nu x_2 + \frac{\mathrm{i}}{2}x_1\cdot\beta x_2,\quad x_1,x_2\in\mathcal{X}. \tag{5.3}$$

Proposition 5.11. *Let $\beta\in L_{\mathrm{a}}(\mathcal{X},\mathcal{X}^\#)$. Then the following are equivalent :*

(1) *β is the covariance of a fermionic quasi-free state ω,*

(2) *$\nu_{\mathbb{C}}+\frac{\mathrm{i}}{2}\beta_{\mathbb{C}}\geq 0$ on $\mathbb{C}\mathcal{X}$,*

(3) $|x_1{\cdot}\beta x_2| \leq 2(x_1{\cdot}\nu x_1)^{\frac{1}{2}}(x_2{\cdot}\nu x_2)^{\frac{1}{2}},\ x_1, x_2 \in \mathcal{X}$.

Proof. as in the bosonic case (1) $\Rightarrow$ (2) and (2) $\Leftrightarrow$ (3) are easy to prove. The proof of (2) $\Rightarrow$ (1) is more difficult, it relies on the Jordan-Wigner representation of $\mathrm{CAR}(\mathcal{X}, \nu)$ for $\mathcal{X}$ finite dimensional. $\Box$

5.7. **Gauge-invariant quasi-free states.** We now assume that $(\mathcal{X}, \nu)$ is equipped with a Kähler anti-involution j. This implies that $\mathrm{e}^{\mathrm{j}\theta} \in U(\mathcal{X}, \nu)$ hence that there exists the group of global gauge transformations τ_θ, $\theta \in [0, 2\pi]$ defined by

$$\tau_\theta \phi(x) := \phi(\mathrm{e}^{\mathrm{j}\theta} x),\ x \in \mathcal{X}.$$

As in the bosonic case, a state ω on $\mathrm{CAR}(\mathcal{X}, \nu)$ is called *gauge invariant* if $\omega \circ \tau_\theta = \omega$, $\forall \theta \in [0, 2\pi]$. Again it is more convenient to use the charged fields :

$$\psi(y) := \phi(y) + \mathrm{i}\phi(\mathrm{j}y),\ \psi^*(y) := \phi(y) - \mathrm{i}\phi(\mathrm{j}y),$$

as generators of $\mathrm{CAR}(\mathcal{Y})$. We recall that one sets $q := 2\nu_{\mathbb{C}} \in L_{\mathrm{h}}(\mathcal{Y}, \mathcal{Y}^*)$, which is more over positive definite.

Proposition 5.12. *A state ω on $\mathrm{CAR}^{C^*}(\mathcal{Y})$ is gauge-invariant quasi-free iff :*

$$\omega\left(\Pi_1^n \psi^*(y_i) \Pi_1^p \psi(x_i)\right) = 0, \textit{ if } n \neq p$$
$$\omega\left(\Pi_1^n \psi^*(y_i) \Pi_1^n \psi(x_i)\right) = \sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) \prod_{i=1}^n \omega(\psi^*(y_i)\psi(x_{\sigma(i)})).$$

Again we can introduce the two complex covariances

$$\omega(\psi(y_1)\psi^*(y_2)) =: \overline{y}_1 \cdot \lambda_+ y_2,\ \omega(\psi^*(y_2)\psi(y_1)) =: \overline{y}_1 \cdot \lambda_- y_2.$$

Proposition 5.13. *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 $\mathrm{CAR}(\mathcal{Y}, q)$,*
(2) *$\lambda_\pm \geq 0$ and $\lambda_+ + \lambda_- = q$.*

5.8. **Pure quasi-free states.** We discuss pure quasi-free states in the fermionic case. We consider the general case, i.e. we do not assume the states to be gauge invariant.

Theorem 5.14. *Let $\beta \in L_{\mathrm{a}}(\mathcal{X}, \mathcal{X}^\#)$. Then β is the covariance of a pure quasi-free state on $\mathrm{CAR}(\mathcal{X}, \nu)$ iff $(\nu, \frac{1}{2}\beta)$ is Kähler, i.e. there exists $\mathrm{j} \in O(\mathcal{X}, \nu)$ such that $\mathrm{j}^2 = -\mathbb{1}$ and $\nu = \frac{1}{2}\beta\mathrm{j}$.*

We leave the formulation of the gauge-invariant version of this theorem as an exercise.

6. Lorentzian manifolds

6.1. **Causality.** Let M a smooth manifold of dimension $n = d + 1$. We assume that M is equipped with a Lorentzian metric g, i.e. a smooth map

$$M \ni x \mapsto g_{\mu\nu}(x) \in L_{\mathrm{s}}(T_x M, T_x^* M),$$

with signature $(-1, d)$. The inverse $g^{-1}(x) \in L_{\mathrm{s}}(T_x^* M, T_x M)$ is traditionally denoted by $g^{\mu\nu}(x)$. We set also $|g|(x) := |\det g_{\mu\nu}(x)|$

Using the metric g we can define time-like, causal, etc. tangent vectors and vector fields on M as on the Minkowski space-time. The set $\{v \in T_xM : vg(x)v = 0\}$ is called the *lightcone* at x.

M is then called *time-orientable* if there exists a global continuous time-like vector field v. Once a time-orientation is chosen, one can define future/past directed time-like vector fields.

One can similarly define time-like, causal etc. piecewise C^1 curves, by requiring the said property to hold for all its tangent vectors.

Definition 6.1. *Let $x \in M$. The* causal*, resp.* time-like future*, resp.* past *of x is the set of all $y \in M$ that can be reached from x by a causal, resp. time-like future-, resp. past-directed curve, and is denoted $J^{\pm}(x)$, resp. $I^{\pm}(x)$. For $\mathcal{U} \subset M$, its* causal*, resp.* time-like future*, resp.* past *is defined as*

$$J^{\pm}(\mathcal{U}) = \bigcup_{x\in\mathcal{U}} J^{\pm}(x), \quad I^{\pm}(\mathcal{U}) = \bigcup_{x\in\mathcal{U}} I^{\pm}(x).$$

We define also the causal*, resp.* time-like shadow *:*

$$J(\mathcal{U}) = J^{+}(\mathcal{U}) \cup J^{-}(\mathcal{U}), \quad I(\mathcal{U}) = I^{+}(\mathcal{U}) \cup I^{-}(\mathcal{U}).$$

The classification of tangent vectors in T_xM can be naturally extended to linear subspaces of T_xM.

Definition 6.2. *A linear subspace E of T_xM is* space-like *if it contains only space-like vectors,* time-like *if it contains both space-like and time-like vectors, and* null *(or* light-like*) if it is tangent to the lightcone at x.*

If $E \subset T_xM$ we denote by $E^{\perp} \subset T_xM$ its orthogonal for $g(x)$.

Lemma 6.3. *A subspace $E \subset T_xM$ is space-like, resp. time-like, resp. null iff $E^{\perp}$ is time-like, resp. space-like, resp. null*

We refer to [F, Lemma 3.1.1] for the proof.

6.2. **Globally hyperbolic manifolds.**

Definition 6.4. *A* Cauchy hypersurface *is a hypersurface $\Sigma \subset M$ such that each inextensible time-like curve intersects Σ at exactly one point.*

The following deep result is originally due to Geroch, with a stronger condition instead of (1b), in this form it is due to Bernal-Sanchez.

Theorem 6.5. *Let M be a connected Lorentzian manifold. The following are equivalent :*

(1) *The following two conditions hold :*
   - *(1a) for any $x, y \in M$, $J^{+}(x) \cap J^{-}(y)$ is compact,*
   - *(1b)* (causality condition) *there are no closed causal curves.*

(2) *There exists a Cauchy hypersurface.*

(3) *M is isometric to $\mathbb{R}\times\Sigma$ with metric $-\beta \mathrm{d}t^2 + g_t$, where β is a smooth positive function, g_t is a Riemannian metric on Σ depending smoothly on $t \in \mathbb{R}$, and each $\{t\} \times \Sigma$ is a smooth space-like Cauchy hypersurface in M.*

Definition 6.6. *A connected Lorentzian manifold satisfying the equivalent conditions of the above theorem is called* globally hyperbolic.

The adjective 'hyperbolic' comes from the connection with hyperbolic partial differential equations : roughly speaking globally hyperbolic space-times are those on which the Cauchy problem for the Klein-Gordon equation can be formulated and uniquely solved.

Definition 6.7. *A function $f : M \to \mathbb{C}$ is called* space-compact *if there exists $K \Subset M$ such that* $\mathrm{supp} f \subset J(K)$. *It is called* future/past space-compact *if there exists $K \Subset M$ such that* $\mathrm{supp} f \subset J^{\pm}(K)$. *The spaces of such smooth functions are denoted by $C^\infty_{\rm sc}(M)$, resp. $C^\infty_{\pm{\rm sc}}(M)$.*

7. Klein-Gordon fields on Lorentzian manifolds

7.1. **The Klein-Gordon operator.** Let (M, g) a Lorentzian manifold. The *Klein-Gordon* operator on M is :

$$P(x, \partial_x) = -|g|^{-\frac{1}{2}}\partial_\mu |g|^{\frac{1}{2}} g^{\mu\nu}(x)\partial_\nu + r(x),$$

acting on functions $u : M \to \mathbb{R}$. Here $r \in C^\infty(M, \mathbb{R})$ represent a (variable) mass. Using the metric connection, one can write

$$P(x, \partial_x) = -\nabla_a \nabla^a + r(x).$$

One can generalize the Klein-Gordon operator to sections of vector bundles, the most important example being the bundle of $1-$forms on M, which appears in the quantization of Maxwell's equation. One would like to interpret some space of smooth solutions of the Klein-Gordon equation :

$$P(x, \partial_x)u = 0 \qquad \text{(KG)}$$

as a symplectic space. Following the discussion in Sect. 5 we will consider *complex* solutions.

7.2. **Conserved current.**

Definition 7.1. *We set for $u_1, u_2 \in C^\infty(M)$:*

$$J^a(u_1, u_2) := \overline{u}_1 . \nabla^a u_2 - \overline{\nabla^a u_1} u_2 \in C^\infty(M)$$

$J^a(u_1, u_2)$ is a vector field, called a *current* in the physics literature. Using the rules to compute with connections we obtain :

$$\begin{aligned} \nabla_a J^a(u_1, u_2) &= \nabla_a \overline{u}_1 \nabla^a u_2 + \overline{u}_1 \nabla_a \nabla^a u_2 - \nabla_a \nabla^a \overline{u}_1 u_2 - \nabla^a \overline{u}_1 \nabla_a u_2 \\ &= \overline{u}_1 \nabla_a \nabla^a u_2 - \nabla_a \nabla^a \overline{u}_1 u_2 = P\overline{u}_1 u_2 - \overline{u}_1 P u_2. \end{aligned}$$

It follows that if $Pu_i = 0$ the vector field $J^a(u_1, u_2)$ is divergence free. Moreover from Gauss formula we obtain :

Lemma 7.2 (Green's formula)**.** *Let $U \subset M$ an open set with ∂U non characteristic. Then*

$$\int_U \overline{u}_1 P u_2 - \overline{Pu}_1 u_2 d\mu_g = -\int_{\partial U} \left(\overline{u}_1 \nabla_a u_2 - \overline{\nabla_a u_1} u_2\right) n^a d\sigma_g.$$

7.3. **Advanced and retarded fundamental solutions.** The treatment of the Klein-Gordon operator is quite similar to its Riemannian analog, i.e. the Laplace operator and starts with the construction of *fundamental solutions*, i.e. inverses. An important difference is the hyperbolic nature of the Klein-Gordon operator : to obtain a unique solution of the equation

$$Pu = v$$

say for $v \in C_0^\infty(M)$, one has to impose extra *support conditions* on u, since there exists plenty of solutions of $Pu = 0$. The condition that (M, g) is globally hyperbolic is the natural condition to be able to construct fundamental solutions. In the sequel we will assume that (M, g) is globally hyperbolic.

The main result is the following theorem, due to Leray.

Theorem 7.3. *For any $v \in C_0^\infty(M)$, there exist unique functions $u^\pm \in C_{\pm\mathrm{sc}}^\infty(M)$ that solve*

$$P(x, \partial_x)u^\pm = v.$$

Moreover,

$$u^\pm(x) = (E^\pm v)(x) := \int E^\pm(x, y)v(y)\mathrm{d}\mu_g(y),$$

where $E^\pm \in \mathcal{D}'(M \times M, L(\mathcal{V}))$ satisfy

$$P \circ E^\pm = E^\pm \circ P = \mathbb{1}, \quad \mathrm{supp}E^\pm \subset \big\{(x, y) \ : \ x \in J^\pm(y)\big\}.$$

Note that P is selfadjoint for the scalar product

$$(u|v) = \int_M \overline{u}v d\mu_g,$$

which by uniqueness implies that $(E^\pm)^* = E^\mp$. This also implies that by duality $E^\pm$ can be applied to distributions of compact support.

Definition 7.4. *E^+, resp. E^-, is called the* retarded*, resp.* advanced Green's function*.*

$$E := E^+ - E^-$$

is called the Pauli-Jordan function*.*

Note that $E = -E^*$, ie. E is anti-hermitian.

7.4. **Cauchy problem.** Once the existence of $E^\pm$ is established, it is easy to solve the Cauchy problem (One can also go the other way around). Let us denote by $\mathrm{Sol}_{\mathrm{sc}}(KG)$ the space of smooth, space compact solutions of (KG). Let Σ be a smooth Cauchy hypersurface. We denote by $\rho : C_{\mathrm{sc}}^\infty(M) \to C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma)$ the map :

$$\rho u := (\rho_0 u, \rho_1 u) = (u_{|\Sigma}, n^\mu \partial_\mu u)_{|\Sigma}).$$

Theorem 7.5. *Let $f \in C_0^\infty(\Sigma) \otimes \mathbb{C}^2$. Then there exists a unique $u \in \mathrm{Sol}_{\mathrm{sc}}(KG)$ such that $\rho u = f$. It satisfies* $\mathrm{supp}u \subset J(\mathrm{supp}f_0 \cup \mathrm{supp}f_1)$ *and is given by*

$$u(x) = -\int_\Sigma n^\mu \nabla_{y^\mu} E(x, y) f_0(y) d\sigma(y) + \int_\Sigma E(x, y) f_1(y) \mathrm{d}\sigma(y). \tag{7.1}$$

We will set $u =: Uf$, for u given by (7.1).

Remark 7.6. *Let us denote by* $\rho_i^* : \mathcal{D}'(\Sigma) \to \mathcal{D}'(M)$ *the adjoints of* ρ_i*. Let us also set*

$$q_\Sigma = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \in L(C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma)).$$

Then (7.1) can be rewritten as :

$$\mathbb{1} = E\rho^* q_\Sigma \rho, \ \textit{on } \mathrm{Sol}_{\mathrm{sc}}(KG), \tag{7.2}$$

or equivalently

$$U = E \circ \rho^* \circ q_\Sigma, \ \textit{on } C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma). \tag{7.3}$$

Proof. We will just prove that the solution u of the Cauchy problem is given by the above formula. We fix $f \in C_0^\infty(M)$ and apply Green's formula to $u_1 = E^\mp f$, $u_1 = u$, and $U = J^\pm(\Sigma)$. We obtain :

$$\begin{aligned} \int_{J^+(\Sigma)} \overline{f} u d\mu_g = &\int_\Sigma \left(\overline{E^- f} \nabla_a u - \overline{\nabla_a E^- f} u\right) n^a d\sigma_g, \\ \int_{J^-(\Sigma)} \overline{f} u d\mu_g = &\int_\Sigma - \left(\overline{E^+ f} \nabla_a u - \overline{\nabla_a E^+ f} u\right) n^a d\sigma_g, \end{aligned}$$

Summing these two identities we obtain :

$$\int_M \overline{f} u d\mu_g = \int_\Sigma \left(-\overline{Ef} \nabla_a u + \overline{\nabla_a E f} u\right) d\sigma_g$$

To complete the proof of the formula, it suffices to introduce the distribution kernel $E(x, y)$ to express Ef as an integral and to use that $E = -E^*$. Details are left to the reader. □

7.5. **Symplectic structure of the space of solutions.** By Thm. 7.5 we know that :

$$\rho : \mathrm{Sol}_{\mathrm{sc}}(KG) \to C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma),$$

is bijective, with inverse U. For $u, v \in \mathrm{Sol}_{\mathrm{sc}}(KG)$ with $\rho u =: f$, $\rho v =: g$ we set :

$$\begin{aligned} &\overline{u_1} \cdot \sigma u_2 := \int_\Sigma \overline{f}_1 g_0 - \overline{f}_0 g_1 d\sigma_g = \int_\Sigma J^a(u, v) n_a d\sigma_g \\ &\overline{f} \sigma_\Sigma g := \int_\Sigma \overline{f}_1 g_0 - \overline{f}_0 g_1 d\sigma_g. \end{aligned} \tag{7.4}$$

It is obvious from Thm. 7.5 that $(\mathrm{Sol}_{\mathrm{sc}}(KG), \sigma)$ is a (complex) symplectic space. From Gauss formula we know that σ is independent on the choice of the Cauchy surface Σ.

7.6. **Space-time fields.**

Theorem 7.7. (1) *consider* $E : C_0^\infty(M) \to C^\infty(M)$*. Then* $\mathrm{Ran} E = \mathrm{Sol}_{\mathrm{sc}}(KG)$*,* $\mathrm{Ker} E = P C_0^\infty(M)$*.*

(2) *One has*

$$\overline{Ef}_1 \cdot \sigma E f_2 = -(f_1 | E f_2), \ f_i \in C_0^\infty(M).$$

Part 1) of the theorem can be nicely rephrased by saying that the sequence :

$$0 \longrightarrow C_0^\infty(M) \xrightarrow{P} C_0^\infty(M) \xrightarrow{E} \mathrm{Sol}_{\mathrm{sc}}(KG) \xrightarrow{P} 0$$

is exact.

Proof. 1) : since $PE^\pm = \mathbb{1}$, we have $PE = 0$, and taking adjoints also $EP = 0$. This shows that $EC_0^\infty(M) \subset \mathrm{Sol}_{\mathrm{sc}}(KG)$ and $PC_0^\infty(M) \subset \mathrm{Ker} E$. It remains to prove the converse inclusions :

1a) $\mathrm{Sol}_{\mathrm{sc}}(KG) \subset EC_0^\infty(M)$: let $u \in \mathrm{Sol}_{\mathrm{sc}}(KG)$. Since u is space-compact, we can find cutoff functions $\chi^\pm \in C^\infty_{\pm\mathrm{sc}}(M)$ such that $\chi^+ + \chi^- = 1$ on $\mathrm{supp}u$. We have some compact sets $K \subset K_1 \subset K_2$ such that $\mathrm{supp}u \subset J(K)$, $\mathrm{supp}\chi^\pm \subset J^\pm(K_2)$, and $\chi^\pm = 1$ on $J^\pm(K_1)$. It follows that $\mathrm{supp}\nabla\chi^\pm \subset J^\pm(K_2)\backslash J^\pm(K_2)$, hence $\mathrm{supp}\nabla\chi^\pm \cap \mathrm{supp}u \subset J^\mp(K_2) \cap J^\pm(K)$. This set is compact by the global hyperbolicity of M.

We set now $u^\pm = \chi^\pm u$, $f = Pu^+ = -Pu^-$. By the above discussion $f \in C_0^\infty(M)$ hence $u^\pm = \pm E^\pm f$ and $u = u^+ + u^- = Ef$.

1b) $\mathrm{Ker}E = PC_0^\infty(M)$: let $u \in C_0^\infty(M)$ such that $Eu = 0$ and let $f = E^\pm u$. Then $\mathrm{supp}f \subset J^+(\mathrm{supp}u) \cap J^-(\mathrm{supp}u)$, hence again by global hyperbolicity, $f \in C_0^\infty(M)$.

2) : from (7.2) we obtain :

$$E = -E\rho^* q_\Sigma \rho E = (\rho \circ E)^* \circ q_\Sigma \circ (\rho \circ E).$$

This implies (2). $\Box$

We now summarize the discussion as follows :

Theorem 7.8. (1) *the following spaces are symplectic spaces :*

$$(C_0^\infty(M)/PC_0^\infty(M), -E),\ (\mathrm{Sol}_{\mathrm{sc}}(KG), \sigma),\ (C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma), \sigma_\Sigma).$$

(2) *the following maps are symplectomorphisms :*

$$(C_0^\infty(M))/PC_0^\infty(M), -E) \xrightarrow{E} (\mathrm{Sol}_{\mathrm{sc}}(KG), \sigma) \xrightarrow{\rho} (C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma), \sigma_\Sigma).$$

7.7. **Quasi-free states for the free Klein-Gordon field.** We can now consider quasi-free states on any of the symplectic spaces in Thm. 7.8. The most natural one is

$$(C_0^\infty(M))/PC_0^\infty(M), E)$$

which leads to *space-time fields*. The associated CCR algebra will be denoted simply by $\mathrm{CCR}(C_0^\infty(M), E)$, ignoring the need to pass to quotient to get a true symplectic space.

Strictly speaking we would write symbols like

$$\phi([f]),\ [f] \in C_0^\infty(M)/PC_0^\infty(M).$$

We write this as

$$\phi(f)\text{''} = \text{''} \int_M \phi(x) f(x) \mathrm{d}\mu_g\text{''} = \text{''}\langle\phi, f\rangle$$

if $P\phi(x) = 0$, i.e. the quantum field ϕ satisfies the KG equation.

causality : denoting by $\phi(f)$ the (selfadjoint) fields associated to $[f] \in C_0^\infty(M))/PC_0^\infty(M)$, we have

$$[\phi(f), \phi(g)] = \mathrm{Re}(f|Eg) = 0,$$

if $\mathrm{supp}f$, $\mathrm{supp}g$ are *causally disjoint*. This follows from the fact that $\mathrm{supp}E(x,y) \subset \{(x,y) \in M \times M\ :\ x \in J(y)\}$.

Let us now consider a gauge-invariant quasi-free state ω, defined by the complex covariances $(\lambda_\pm)$. Recall that $\lambda_\pm$ are sesquilinear forms on $C_0^\infty(M))/PC_0^\infty(M)$. One may assume that they are obtained from sesquilinear forms $\Lambda_\pm$ on $C_0^\infty(M)$ which pass to quotient, i.e. such that :

$$P^* \circ \Lambda_\pm = \Lambda_\pm \circ P = 0. \tag{7.5}$$

It is also natural to assume that $\Lambda_{\pm}$ are continuous sesquilinear forms, hence by the Schwartz kernel theorem have distributional kernels $\Lambda_{\pm}(x,y) \in \mathcal{D}'(M \times M)$. Then (7.5) becomes, using that $P = P^*$:

$$P(x, \partial_x)\Lambda_{\pm}(x,y) = P(y, \partial_y)\Lambda_{\pm}(x,y) = 0. \tag{7.6}$$

8. Free Dirac fields on Lorentzian manifolds

8.1. **The Dirac operator.** Let (M, g) be a Lorentzian manifold. To define correctly a Dirac operator we need a *spin structure*. We keep the discussion simple, and use a framework in [DG], assuming that the manifold M is parallelizable.

Let $\mathcal{V}$ be a complex, finite dimensional vector space. We assume that there exists a map $M \ni x \mapsto \gamma^a(x) \in L(\mathcal{V})$ such that

$$[\gamma^a(x), \gamma^b(x)]_+ = 2g^{ab}(x)$$

Of course to make this definition clean one should use the language of bundles. One can think of γ^a as x dependent Dirac matrices.

Definition 8.1. *Let $M \ni x \mapsto m(x) \in L(\mathcal{V})$. The operator on $C^\infty(M; \mathcal{V})$*

$$\mathbb{D} := \gamma^a \partial_{x^a} + m(x)$$

is called a Dirac operator *on M. The* Dirac equation *is :*

$$\mathbb{D}\zeta = 0. \tag{D}$$

We need some more structure to be able to quantize the Dirac equation. We assume that there exists a smooth map :

$$M \ni x \mapsto \lambda(x) \in L_{\rm h}(\mathcal{V}, \mathcal{V}^*) \tag{8.7}$$

such that :

$$\begin{aligned} &\gamma^a(x) \text{ is selfadjoint for } \lambda(x), \\ &m(x) - \tfrac{1}{2}\nabla_a \gamma^a(x) \text{ is anti-selfadjoint for } \lambda(x). \end{aligned} \tag{8.8}$$

We equip $C_0^\infty(M; \mathcal{V})$ of the sesquilinear form

$$(\zeta_1|\zeta_2) = \int_M \overline{\zeta}_1(x) \cdot \lambda(x)\zeta_2(x) d\mu_g,$$

and we obtain that if (8.8) holds then $\mathbb{D}^* = -\mathbb{D}$.

8.2. **Conserved current.** We set for $\zeta_1, \zeta_2 \in C^\infty(M; \mathcal{V})$

$$J^a(\zeta_1, \zeta_2) := \overline{\zeta}_1(x) \cdot \lambda(x)\gamma^a(x)\zeta_2(x).$$

One proves that if ζ_i are solutions of the Dirac equation, then

$$\nabla_a J^a(\zeta_1, \zeta_2) = 0.$$

We also get the Green's formula :

Lemma 8.2. *Let $U \subset M$ an open set with ∂U non characteristic. Then*

$$\int_U \overline{\zeta}_1 \cdot \lambda \mathbb{D}\zeta_2 - \overline{\mathbb{D}\zeta}_1 \cdot \lambda \zeta_2 d\mu_g = -\int_{\partial U} \overline{\zeta}_1 \cdot \lambda \gamma_a \zeta_2 n^a d\sigma_g,$$

for $\gamma_a = g_{ab}\gamma^b$.

8.3. **Advanced and retarded fundamental solutions.** We assume now that (M, g) is globally hyperbolic. It is easy to construct fundamental solutions for the Dirac operator : in fact $\mathbb{D}\mathbb{D}$ is a Klein-Gordon operator, acting on vector valued functions, but with scalar principal part equal to $-\nabla_a \nabla^a$. The existence of fundamental solutions $E^{\pm}$ for $\mathbb{D}^2$ yields the fundamental solutions $S^{\pm} = \mathbb{D}E^{\pm}$. This is summarized in the next theorem.

Theorem 8.3. *For any $f \in C_0^\infty(M; \mathcal{V})$, there exist unique functions $\zeta^{\pm} \in C^\infty_{\pm \mathrm{sc}}(M; \mathcal{V})$ that solve*

$$\mathbb{D}\zeta^{\pm} = f.$$

Moreover,

$$\zeta^{\pm}(x) = (S^{\pm}f)(x) := \int S^{\pm}(x, y) f vy) \mathrm{d}\mu_g(y),$$

where $S^{\pm} \in \mathcal{D}'(M \times M, L(\mathcal{V}))$ satisfy

$$\mathbb{D} \circ S^{\pm} = S^{\pm} \circ \mathbb{D} = \mathbb{1}, \quad \mathrm{supp} S^{\pm} \subset \big\{(x, y) \ : \ x \in J^{\pm}(y)\big\}.$$

If (8.8) holds then

$$\lambda(x) S^{\pm}(x, y) = -S^{\mp}(x, y)^* \lambda(y),$$

i.e. $S^{\pm *} = -S^{\mp}$, if we equip $C_0^\infty(M; \mathcal{V})$ with the (non-positive) scalar product obtained from λ.

Definition 8.4. *$S^{\pm}$ are called the* retarded/advanced *Green's functions.*

$$S := S^+ - S^-$$

is called the Pauli-Jordan *function.*

Note that $S = S^*$, i.e. S is hermitian.

8.4. **Cauchy problem.** We state without proof the existence and uniqueness result for the Cauchy problem. We denote by $\rho : C^\infty_{\mathrm{sc}}(M; \mathcal{V}) \to C_0^\infty(\Sigma; \mathcal{V})$ the trace on Σ and by $\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D})$ the space of smooth space-compact solutions of the Dirac equation.

Theorem 8.5. *Let Σ be a Cauchy surface. Then for any $f \in C_0^\infty(\Sigma; \mathcal{V})$ there exists a unique $\zeta \in \mathrm{Sol}_{\mathrm{sc}}(\mathbb{D})$ such that $\rho\zeta = f$. It satisfies* $\mathrm{supp}\zeta \subset J(\mathrm{supp} f)$ *and is given by :*

$$\zeta(x) = -\int_\Sigma S(x, y) \gamma^a(y) n_a(y) f(y) d\mu_g(y).$$

8.5. **Hermitian structure on the space of solutions.** We would like to equip $\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D})$ with a (positive) hermitian structure. To do this we need an additional positivity condition. We assume that there exists a global, time-like future directed vector field v such that

$$\lambda(x)\gamma^a(x)v_a(x) > 0,\ \forall x \in M. \tag{8.9}$$

It can be shown that if this is true for one such vector field, it is automatically true for all such vector fields, in particular for the normal vector to a given Cauchy surface. For $\zeta_1, \zeta_2 \in \mathrm{Sol}_{\mathrm{sc}}(\mathbb{D})$ with $\rho\zeta_i = f_i$ we set :

$$\begin{aligned} \overline{\zeta}_1 \cdot \nu\zeta_2 &:= \int_\Sigma J^a(\zeta_1, \zeta_2)n_a d\sigma_g = \int_\Sigma \overline{f}_1 \cdot \lambda(y)\gamma^a(y)f_2(y)n_a(y)d\sigma_g(y), \\ \overline{f}_1 \cdot \nu_\Sigma f_2 &= \int_\Sigma \overline{f}_1 \cdot \lambda(y)\gamma^a(y)f_2(y)n_a(y)d\sigma_g(y). \end{aligned} \tag{8.10}$$

From Thm. 8.5 we see that $(\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}), \nu)$ is a hermitian space, and from (8.9) ν is positive definite. Moreover from Gauss formula ν is independent on the choice of a Cauchy surface.

8.6. **Space-time fields.**

Theorem 8.6. (1) *consider* $S : \mathcal{D}(M; \mathcal{V}) \to C^\infty(M; \mathcal{V})$. *Then* $\mathrm{Ran}S = \mathrm{Sol}_{\mathrm{sc}}(\mathbb{D})$ *and* $\mathrm{Ker}S = \mathbb{D}C_0^\infty(M; \mathcal{V})$.

(2) *One has :*

$$\overline{Sf}_1 \cdot \nu S f_2 = (f_1|Sf_2),\ f_i \in C_0^\infty(M; \mathcal{V}).$$

Proof. 1) is left to the reader.

2) : Thm. 8.5 can be rewritten as

$$\mathbb{1} = S\rho^*\gamma^{a*}n_a\rho, \text{ on } \mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}),$$

hence by 1)

$$S = S\rho^*\gamma^{a*}n_a\rho S,$$

which implies 2) since $S^* = S$. □

Theorem 8.7. (1) *the following spaces are pre-Hilbert spaces :*

$$(C_0^\infty(M; \mathcal{V})/\mathbb{D}C_0^\infty(M; \mathcal{V}), S),\ (\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}), \nu),\ (C_0^\infty(\Sigma; \mathcal{V}), \nu_\Sigma).$$

(2) *the following maps are unitary :*

$$(C_0^\infty(M; \mathcal{V})/\mathbb{D}C_0^\infty(M; \mathcal{V}), S) \xrightarrow{S} (\mathrm{Sol}_{\mathrm{sc}}(\mathbb{D}), \nu) \xrightarrow{\rho} (C_0^\infty(\Sigma; \mathcal{V}), \nu_\Sigma).$$

8.7. **Quasi-free states for the free Dirac field.** As for the Klein-Gordon case we choose the pre-Hilbert space :

$$(C_0^\infty(M; \mathcal{V})/\mathbb{D}C_0^\infty(M; \mathcal{V}), S).$$

The associated CAR algebra is denoted by $\mathrm{CAR}(C_0^\infty(M; V), S)$.

The causality is a bit different : we obtain

$$[\phi(f), \phi(g)]_+ = \mathrm{Re}(f|Sg) = 0,$$

if $\mathrm{supp}f$, $\mathrm{supp}g$ are *causally disjoint*, i.e. fields supported in causally disjoint regions *anti-commute*. This puzzle is solved by considering only *even* elements of $\mathrm{CAR}(C_0^\infty(M; \mathcal{V})/\mathbb{D}C_0^\infty(M; \mathcal{V}), S)$ as true physical observables.

Let us consider a gauge-invariant quasi-free state ω, defined by the complex covariances $(\lambda_\pm)$. Recall that $\lambda_\pm$ are sesquilinear forms on $C_0^\infty(M;\mathcal{V})/\mathbb{D}C_0^\infty(M;\mathcal{V}))$. Again one assumes that they are obtained from sesquilinear forms $\Lambda_\pm$ on $C_0^\infty(M;\mathcal{V})$ which pass to quotient, i.e. such that :

$$\mathbb{D}\circ\Lambda_\pm = \Lambda_\pm\circ\mathbb{D} = 0. \tag{8.11}$$

Introducing as before the distributional kernels $\Lambda_\pm(x,y)\in\mathcal{D}'(M\times M)\otimes\mathcal{V}\otimes\mathcal{V}^*$. Then (8.11) becomes :

$$\mathbb{D}(x,\partial_x)\Lambda_\pm(x,y) = \mathbb{D}(y,\partial_y)\Lambda_\pm(x,y) = 0. \tag{8.12}$$

9. Microlocal analysis of Klein-Gordon quasi-free states

9.1. **The need for renormalization.** The stress -energy tensor for a classical Klein-Gordon field is given by :

$$T_{\mu\nu}(x) = \nabla_\mu\phi(x)\nabla_\nu\phi(x) - \frac{1}{2}g_{\mu\nu}(x)\left(g_{ab}(x)\nabla_a\phi(x)\nabla_b\phi(x) - m^2\phi^2(x)\right).$$

For a quantized Klein-Gordon field one would like to be able to define $T_{\mu\nu}(x)$ as an operator valued distribution. This means the following :

we choose a state ω (say a quasi-free state), and fix $f_1,\dots,f_n,\ g_1,\dots,g_p\in C_0^\infty(M)$. Then

$$x\mapsto\omega(\prod_1^n\phi(f_i)T_{\mu\nu}(x)\prod_1^p\phi(g_j))$$

should be a distribution on M. This is never the case, even on Minkowski space : for example $\omega(\phi^2(x))$ should be the trace on $x=x'$ of $\omega(\phi(x)\phi(x'))=\omega_2(x,x')$, which makes no sense. We need to subtract the singular part of $\omega_2(x,x')$ near the diagonal, i.e. to perform a renormalization.

Another requirement is that the renormalization procedure should be 'covariant' : it should depend only on the metric in a arbitrarily small neighborhood of x. This implies that is will be covariant under isometric embeddings.

The procedure is as follows. One first performs the 'point-splitting', i.e. consider

$$T^{\mu\nu}(x,y) = \nabla_\mu\phi(x)\nabla_\nu\phi(y) - \frac{1}{2}g_{\mu\nu}(x)\left(g_{ab}(x)\nabla_a\phi(x)\nabla_b\phi(y) - m^2\phi(x)\phi(y)\right).$$

One then remove the singular part by setting :

$$:\phi(x)\phi(y): = \ \phi(x)\phi(y) - c_{\rm Had}(x,y)\mathbb{1},$$

where $c_{\rm Had}(x,y)$ is a well chosen distributional kernel. Then one has to check that the distributions

$$\omega(\prod_1^n\phi(x_i) T_{\mu\nu}(x,y): \prod_1^p\phi(y_j))$$

have well-defined restrictions to $x=y$.

9.2. **Old form of Hadamard states.** Choose a Cauchy surface Σ. A causal normal neighborhood N of Σ in M is an open neighborhood of Σ such that Σ is a Cauchy surface of (N, g) and for each $x, x' \in N$ such that $x \in J^+(x')$ there exists a convex normal open set containing $J^+(x') \cap J^-(x)$. We fix a *time function* $T : M \to \mathbb{R}$, i.e.a smooth function which increases towards the future, and a open neighborhood $\mathcal{O} \subset M \times M$ of the set of pairs of causally related points (x, x') such that $J^\pm(x) \cap J^\mp(x')$ are contained in a convex, normal open neighborhood.

One fixes also $\mathcal{O}'$ an open neighborhood in $N \times N$ of the set of pairs of causally related points such that $\mathcal{O}' \subset \overline{\mathcal{O}}$.

The squared geodesic distance $\sigma(x, x')$ is smooth on $\mathcal{O}$ and well defined on the subset of $N \times N$ consisting of causally related points. The *van Vleck-Morette determinant* is

$$\Delta(x, x') := -\det(-\nabla_\alpha \nabla_{\beta'} \sigma(x, x'))|g|^{-\frac{1}{2}}(x)|g|^{-\frac{1}{2}}(x').$$

One can then construct a sequence of functions $v^{(n)} \in C^\infty(\mathcal{O} \times \mathcal{O})$ of the form

$$v^{(n)}(x, x') = \sum_1^n \sigma(x, x')^i v_i(x, x'),$$

where the $v_i \in C^\infty(\mathcal{O} \times \mathcal{O})$ are uniquely determined by some transport equations (the so-called Hadamard recursion relations).

One then defines a sequence of distributions $c^{(n)}_{\rm Had} \in \mathcal{D}'(\mathcal{O} \times \mathcal{O})$ for $n \geq 1$ by :

$$\begin{aligned} c^{(n)}_{\rm Had}(x, x') = & \ \lim\nolimits_{\epsilon \to 0^+} \frac{(2\pi)^2 \Delta(x, x')^{\frac{1}{2}}}{\sigma(x, x') + 2\mathrm{i}\epsilon(T(x) - T(x')) + \epsilon^2} \\ + & \ \lim\nolimits_{\epsilon \to 0^+} v^{(n)}(x, x') \ln\left(\sigma(x, x') + 2\mathrm{i}\epsilon(T(x) - T(x'))\right). \end{aligned}$$

Let us now give the old definition of Hadamard states, restricting ourselves to real Klein-Gordon fields.

Definition 9.1. *A quasi-free state* ω *on* $\mathrm{CCR}(C_0^\infty(M), E)$ *is a Hadamard state if for any* $m \in \mathbb{N}$ *there exists* $n \in \mathbb{N}$ *such that* $\omega_2 - c^{(n)}_{\rm Had}$ *is of class* C^m *in* $\mathcal{O}'$.

9.3. **The wavefront set on a manifold.** Let M be a manifold, T^*M be the cotangent bundle. The zero section $T^*_0 M$ will be denoted by Z.

We recall the spaces : $\mathcal{D}(M)$ (smooth compactly supported functions), $\mathcal{D}'(M)$ (distributions), $\mathcal{E}(M)$ (smooth functions with well-known topology), $\mathcal{E}'(M)$ (distributions with compact support).

9.4. **Operations on conic sets.** A set $\Gamma \subset T^*M \backslash Z$ is *conic* if $(x, \xi) \in \Gamma \Rightarrow (x, t\xi) \in \Gamma$ for all $t > 0$. Let $\Gamma_i \subset T^*M \backslash Z$, $i = 1, 2$ be conic sets. We set :

$$\begin{aligned} -\Gamma &:= \{(x, -\xi) \ : (x, \xi) \in \Gamma\}, \\ \Gamma_1 \oplus \Gamma_2 &:= \{(x, \xi_1 + \xi_2) \ : \ (x, \xi_i) \in \Gamma_i\}. \end{aligned}$$

Let M_i, $i = 1, 2$ be two manifolds and $\Gamma \subset T^*M_1 \times M_2 \backslash Z$ be a conic set. The elements of $T^*M_1 \times M_2 \backslash Z$ 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 :

$$\begin{aligned}
\Gamma' &:= \{(x_1,\xi_1,x_2,-\xi_2) \ : \ (x_1,\xi_1,x_2,\xi_2)\in\Gamma\},\\
{}_{M_1}\Gamma &:= \{(x_1,\xi_1) \ : \ \exists x_2 \text{ such that } (x_1,\xi_1,x_2,0)\in\Gamma\} = \Gamma(Z_2),\\
\Gamma_{M_2} &:= \{(x_2,\xi_2) \ : \ \exists x_1 \text{ such that } (x_1,0,x_2,\xi_2)\in\Gamma\} = \Gamma^{-1}(Z_1).
\end{aligned}$$

9.5. **Operations on distributions.**

(1) **Complex conjugation** : if $u\in\mathcal{D}'(M)$ then $WF\overline{u} = -WF(u)$.

(2) **Tensor product** : if $u_i\in\mathcal{D}'(M_i)$, $i=1,2$ then

$$\begin{aligned}
& WF(u_1\otimes u_2)\\
\subset\ & (WF(u_1)\times WF(u_2))\cup(\mathrm{supp}u_1\times\{0\})\times WF(u_2)\cup WF(u_1)\times(\mathrm{supp}u_2\times\{0\})\\
\subset\ & (WF(u_1)\times WF(u_2))\cup Z_1\times WF(u_2)\cup WF(u_1)\times Z_2.
\end{aligned}$$

(3) **Restriction to a submanifold** : let $S\subset M$ a submanifold. The conormal bundle T^*_SM is defined as :

$$T^*_SM := \{(x,\xi)\in T^*M\backslash Z \ : \ x\in S, : \xi\cdot v = 0 \ \forall v\in T_xS\}.$$

If $u\in\mathcal{D}'(M)$ the restriction $u_{|S}$ of u to S is well defined if $WFu\cap T^*_SM=\emptyset$. One has

$$WFu_{|S}\subset\{(x,\xi_{|T_xS}) \ : \ x\in S, \ (x,\xi)\in WF(u)\}.$$

(4) **Product** : if $u_i\in\mathcal{D}'(M)$, $i=1,2$ then u_1u_2 is well defined if $WF(u_1)\oplus WF(u_2)\cap Z=\emptyset$ and then :

$$WF(u_1u_2)\subset WF(u_1)\cup WF(u_2)\cup WF(u_1)\oplus WF(u_2).$$

(5) **Kernels** : let $K:\mathcal{D}(M_2)\to\mathcal{D}'(M_1)$ be linear continuous and $K(x_1,x_2)\in\mathcal{D}'(M_1\times M_2)$ its distributional kernel.
then Ku is well defined for $u\in\mathcal{E}'(M_2)$ if $WF(u)\cap WF'_{M_2}(K)=\emptyset$ and then :

$$WF(Ku)\subset \ {}_{M_1}WF(K)\cup WF'(K)\circ WF(u).$$

(6) **Composition** : 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 ie the projection : $\mathrm{supp}K_2\to M_2$ is proper. Then $K_1\circ K_2$ is well defined if :

$$WF'(K_1)_{M_2}\ \cap\ {}_{M_2}WF(K_2)=\emptyset,$$

and then

$$WF'(K_1\circ K_2)\subset WF'(K_1)\circ WF'(K_2)\ \cup\ ({}_{M_1}WF(K_1)\times Z_3)\ \cup\ (Z_1\times WF(K_2)_{M_3}).$$

9.6. **Parametrices for the Klein-Gordon operator.** Once we choose an orientation, we can define for $x \in M$ the open future/past light cones $V_x^{\pm} \subset T_xM$. We denote by $V_{x\pm}^* \subset T_x^*M$ the dual cones

$$V_{x\pm}^* = \{\xi \in T_x^*M \ : \ \xi \cdot v > 0, \ \forall v \in V_{x\pm}, \ v \neq 0\}.$$

For simplicity we write

$$\xi \rhd 0 \text{ (resp. } \xi \lhd 0) \text{ if } \xi \in V_{x+}^* \text{ (resp. } V_{x-}^*).$$

$$\xi \unrhd 0 \text{ (resp. } \xi \unlhd 0) \text{ if } \xi \in (V_{x+}^*)^{\rm cl} \text{ (resp. } (V_{x-}^*)^{\rm cl}).$$

The principal symbol of the Klein-Gordon operator P is $p(x,\xi) = \xi_\mu g^{\mu\nu}(x)\xi_\nu$ and one sets

$$N := p^{-1}(\{0\}) \cap T^*M\backslash Z,$$

called the *characteristic manifold* of P. Note that N splits into its two connected components (positive/negative energy shells) :

$$N = N^+ \cup N^-, \ N^{\pm} = N \cap \{\pm\xi \unrhd 0\}.$$

We denote by H_p the Hamilton field of p. We denote by $X = (x,\xi)$ the points in $T^*M\backslash Z$. The bicharacteristic (Hamilton curve for p) passing through X is denoted by $B(X)$ For $X, Y \in N$ we write $X \sim Y$ if $Y \in B(X)$. Clearly this is an equivalence relation.

For $X \sim Y$, we write $X \succ Y$ (resp. $X \prec Y$) if X comes strictly after (before) Y w.r.t. the natural parameter on the bicharacteristic curve through X and Y.

We recall Hörmander's propagation of singularities theorem :

Theorem 9.2. *Let $u \in \mathcal{D}'(M)$ such that $Pu \in C^\infty(M)$. Then*

$$WF(u) \subset N, \ X \in WF(u) \Rightarrow B(X) \subset WF(u).$$

The *bicharacteristic relation* of P is the set :

$$C := \{(X,Y) \in N \times N \ : \ X \sim Y\}.$$

We set :

$$\Delta_N := \{(X,X)\} \cap N \times N$$

the diagonal in $N \times N$.

Parametrices (i.e. inverses modulo smoothing operators) of operators of real principal type (of which Klein-Gordon operators are an example) were studied by Duistermaat and Hörmander in the famous paper [DH]. They introduced the notion of *distinguished parametrices*, i.e. parametrices which are uniquely determined (modulo smoothing terms of course), by the wavefront set of their kernels. Distinguished parametrices are in one to one correspondence with *orientations* of C, defined below.

Definition 9.3. *An orientation of C is a partition of $C\backslash\Delta_N$ as $C^1 \cup C^2$ where C^i are open sets in $C\backslash\Delta_N$ and inverse relations (ie* $\mathrm{Exch}(C^1) = C^2$*).*

Note that $C^i \neq \emptyset$, $C^i \neq C\backslash\Delta_N$ (because they are inverse relations) and C^i are open and closed in $C\backslash\Delta_N$. Therefore C^i are union of connected components of $C\backslash\Delta_N$.

Theorem 9.4 (D-H)**.** *Let $C\backslash\Delta_N = C^1 \cup C^2$ an orientation of C. Then there exists parametrices E^i, $i = 1, 2$ of P such that :*

$$WF'(E^i) \subset \Delta^* \cup C^i,$$

where Δ^* is the diagonal in $T^*M\backslash Z \times T^*M\backslash Z$. Any left or right parametrix with the same property is equal to E^1 or E^2 modulo C^∞.

Orientations of C are themselves in one to one correspondence to the partitions of $N^1 \cup N^2 = N$ into open and closed sets, ie into connected components of N. For the Klein-Gordon operator N has two connected components :

$$N_\pm := \{X \in N \ : \xi \in V^*_{x\pm}\},$$

which are invariant under the bicharacteristic flow, hence two orientations, hence four distinguished parametrices. The two connected components are N_+, N_-. The two orientations are

$$\begin{aligned} &C\backslash\Delta_N = C^+ \cup C^- \text{ for} \\ &C^+ := \{(X,Y) \in C \ : \ x \in J^+(y)\}, \ C^- := \{(X,Y) \in C \ : \ x \in J^-(y)\} \end{aligned}$$

and

$$\begin{aligned} &C\backslash\Delta_N = C_+ \cup C_- \text{ for} \\ &C_+ := \{(X,Y) \in C \ : \ X \prec Y\}, \ C_- := \{(X,Y) \in C \ : \ X \succ Y\}. \end{aligned}$$

Note that :

$$X \prec Y \ \Leftrightarrow \ X \sim Y \text{ and } \begin{cases} x \in J^+(y), \ X, Y \in N_+, \\ \text{or } x \in J^-(y), \ X, Y \in N_-; \end{cases}$$

$$X \succ Y \ \Leftrightarrow \ X \sim Y \text{ and } \begin{cases} x \in J^-(y), \ X, Y \in N_+, \\ \text{or } x \in J^+(y), \ X, Y \in N_-. \end{cases}$$

The parametrices associated to these orientations are well-known in physics, we have already encountered two of them, namely $E^\pm$.

Feynman : denoted E_F :

$$\mathrm{WF}(E_F)' = \Delta^* \cup C_+$$

anti-Feynman : denoted $E_{\overline{F}}$:

$$\mathrm{WF}(E_{\overline{F}})' = \Delta^* \cup C_-$$

retarded : E^+ :

$$\mathrm{WF}(E^+)' = \Delta^* \cup C^+,$$

advanced : E^- :

$$\mathrm{WF}(E^-)' = \Delta^* \cup C^-.$$

The parametrices $E^\pm$ are more fundamental since they are used to define the symplectic form E. The parametrices E_F, $E_{\overline{F}}$ appear in connection with the vacuum state on Minkowski space, and with Hadamard states on general curved spacetimes.

9.7. **Examples.** Assume that $P = \partial_t^2 + \epsilon^2$ (whatever ϵ^2 is, for example a real number). Then :

$$\begin{aligned} E^+(t) &= \theta(t)\tfrac{\sin \epsilon t}{\epsilon}, \\ E^-(t) &= -\theta(-t)\tfrac{\sin \epsilon t}{\epsilon}, \\ E_F(t) &= \tfrac{1}{2\mathrm{i}\epsilon}\left(\mathrm{e}^{\mathrm{i}t\epsilon}\theta(t) + \mathrm{e}^{-\mathrm{i}t\epsilon}\theta(-t)\right), \\ E_{\overline{F}}(t) &= -\tfrac{1}{2\mathrm{i}\epsilon}\left(\mathrm{e}^{-\mathrm{i}t\epsilon}\theta(t) + \mathrm{e}^{\mathrm{i}t\epsilon}\theta(-t)\right), \end{aligned}$$

for $\theta(t)$ =Heaviside function.

We prove some properties of the distinguished parametrices.

Lemma 9.5. *We have :*

$$\begin{aligned} &1) \quad WF'(E^+ - E^-) = C, \\ &2) \quad WF'(E_F - E^+) = C \cap N_- \times N_-, \\ &3) \quad WF'(E_F - E^-) = C \cap N_+ \times N_+. \end{aligned}$$

Proof.

1) : since E^+ and E^- have disjoint wave front sets above $\{x_1 \neq x_2\}$, we see that above $\{x_1 \neq x_2\}$

$$WF'(E^+ - E^-) = WF'(E^+) \cup WF'(E^-) = C \backslash \Delta_N.$$

Since $P_1(E^+ - E^-) \in C^\infty$ by propagation of singularities we obtain that $\Delta_N \subset WF'(E^+ - E^-)$. This proves 1).

2) : above $\{(x_1, x_2) \ : \ x_1 \in J^-(x_2)\}$ we have

$$WF'(E_F - E^+) = WF'(E_F) = \{(X_1, X_2) \ : \ x_1 \in J^-(x_2), \xi_1 \lhd 0\}.$$

Using again that $P_1(E^+ - E_F) \in C^\infty$ we obtain that $WF'(E_F - E^+) = C \cap N_- \times N_-$. The proof of 3) is similar. □

9.8. **The theorem of Radzikowski.**

Definition 9.6. *Let $\Lambda_\pm : \mathcal{D}(M) \to \mathcal{E}(M)$ be linear continuous. The pair $\Lambda_\pm$ satisfies the* Hadamard condition *if :*

$$(Had)\ \mathrm{WF}(\Lambda_\pm)' = \{(X_1, X_2) \in N^\pm \times N^\pm : \ X_1 \sim X_2\}.$$

The pair $\Lambda_\pm$ satisfies the generalized Hadamard condition *if there exists conic sets $\Gamma_\pm$ with $(X_1, X_2) \in \Gamma_\pm \Rightarrow \pm\xi_1 \rhd 0, \pm\xi_2 \rhd 0$ such that*

$$(genHad)\ \ WF(\Lambda_\pm)' \subset \Gamma_\pm.$$

We introduce the following conditions on a pair $\Lambda_\pm$:

$$(KG)\ P \circ \Lambda_\pm, \Lambda_\pm \circ P \text{ smoothing},$$

$$(CCR)\ \Lambda_+ - \Lambda_- - \mathrm{i}E \text{ smoothing}$$

The following theorem is the theorem of Radzikowski (extended to the complex case).

Theorem 9.7. *The following three conditions are equivalent :*

(1) $\Lambda_\pm$ *satisfy (Had), (KG) and (CCR),*
(2) $\Lambda_\pm$ *satisfy (genHad), (KG) and (CCR),*

(3) *one has :*

$$\Lambda_{\pm} = \mathrm{i}(E_F - E_{\mp}) \text{ modulo } C^\infty(M \times M).$$

Proof. (1) $\Rightarrow$ (2) : obvious.

(2) $\Rightarrow$ (3) : set $S_{\pm} = \mathrm{i}(E_F - E_{\mp})$ By Lemma 9.5 we have $\mathrm{WF}(S_{\pm})' \subset C \cap (N_{\pm} \times N_{\pm})$. By (KG) and Thm. 9.2 we obtain that $\mathrm{WF}(\Lambda_{\pm})' \subset N \times N$. Using then (genHad) we obtain that $\mathrm{WF}(\Lambda_{\pm}) \subset \Gamma_{\pm} \cap N \times N \subset N_{+} \times N_{+}$. This implies that

$$\mathrm{WF}(\Lambda_{\pm} - S_{\pm})' \subset N_{\pm} \times N_{\pm},$$

which implies in particular that

$$\mathrm{WF}(\Lambda_{+} - S_{+})' \cap \mathrm{WF}(\Lambda_{-} - S_{-})' = \emptyset. \tag{9.1}$$

By (CCR) we have also

$$(\Lambda_{+} - S_{+}) - (\Lambda_{-} - S_{-}) = \mathrm{i}E - (S_{+} - S_{-}) = \mathrm{i}E - \mathrm{i}E \text{ mod } C^\infty(M \times M).$$

By (9.1) this implies that both $\Lambda_{\pm} - S_{\pm}$ are smooth.

(3) $\Rightarrow$ (1) : (KG) and (CCR) are obvious, (Had) follows from Lemma 9.5. □

There is a remaining painful step, which I will only briefly explain. I will consider real fields for simplicity. The conclusion of the above theorem for the real covariance $\omega_2(x, x')$ is that $\omega_2 = \mathrm{i}(E_F - E^{+})$ mod C^∞. Then one has to perform some painful computations to prove that $\mathrm{i}(E_F - E^{+}) = c_{\mathrm{Had}}$ mod C^∞.

9.9. **Return to the stress-energy tensor.** Let us forget the derivatives and juste consider $:\phi^2(x):$. We put just one field on each side (extension to several fields is straightforward) :

We compute the expectation value of

$$\phi(x_1)\phi(x)\phi(y)\phi(x_2) - \phi(x_1)\phi(x_2)c_{Had}(x, x'),$$

in the state ω. By the quasi-free property, we obtain a sum of two types of terms :

$$\omega_2(x_1, x)\omega_2(x', x_2),\ \omega_2(x, x_2)\omega_2(x_1, x'),$$

and

$$\omega_2(x_1, x_2) \times (\omega_2(x, x') - c_{Had}(x, x')).$$

The second term has a restriction to the diagonal $x = x'$, since $\omega_2 - c_{Had}$ is smooth.

For the first term we consider the wavefront set of the distribution. By the tensor product rule we obtain :

$$\mathrm{WF}(\omega_2) \times \mathrm{WF}(\omega_2) \cup (\mathrm{supp}\omega_2 \times \{0\}) \times \mathrm{WF}(\omega_2) \cup \mathrm{WF}(\omega_2) \times (\mathrm{supp}\omega_2 \times \{0\}).$$

We compute the conormal to $S = \{x = x'\}$:

$$T^*_S M = \{(x_1, \xi_1, x, \xi, y, \eta, x_2, \xi_2) \ :\ \xi_1 = \xi_2 = 0,\ x = y,\ \xi = -\eta\}$$

We have to show the intersection is empty, which is obvious since $(X, Y) \in WF(\omega_2)$ implies $\xi, \eta \neq 0$.

10. Construction of Hadamard states

It is not a priori obvious that Hadamard states exist on an arbitrary globally hyperbolic spacetime. In this section we explain some constructions of Hadamard states.

10.1. **Ultrastatic spacetimes.** Consider an ultrastatic spacetime $(\mathbb{R}\times\Sigma, g)$, $g = -dt^2 + h$. Let $a = -\Delta_h + m^2$ on Σ and $\epsilon = a^{\frac{1}{2}}$. One can then define the *vacuum state* $\omega_{\rm vac}$, whose two-point function is given by the kernel :

$$\Lambda_{\pm}^{\rm vac}(t) = \frac{1}{2\epsilon}{\rm e}^{\pm {\rm i}t\epsilon},$$

i.e. writing $u \in C^\infty(\mathbb{R}\times\Sigma)$ as $\mathbb{R} \ni t \mapsto u(t) \in C^\infty(\Sigma)$:

$$\Lambda_{\pm}^{\rm vac}u(t) = \int_{\mathbb{R}} \frac{1}{2\epsilon}{\rm e}^{\pm {\rm i}(t-s)\epsilon}u(s)ds.$$

Sahlmann and Verch [SV] have shown that $\omega_{\rm vac}$ is a Hadamard state. Another proof can be given by using the arguments of Subsect. 10.3.

Similarly one can define the *thermal state* at temperature β^{-1}, $\beta > 0$ with kernel

$$\Lambda_{\pm}^{\beta}(t) := \frac{1}{2\epsilon(1-{\rm e}^{-\beta\epsilon})}({\rm e}^{\pm {\rm i}t\epsilon} + {\rm e}^{\mp {\rm i}t\epsilon}{\rm e}^{-\beta\epsilon}).$$

It is again a Hadamard state since ${\rm e}^{-\beta\epsilon}$ is a smoothing operator

The conclusion is that vacuum or thermal states on ultrastatic (or static) spacetimes are Hadamard states.

10.2. **The FNW deformation argument.** Let (M, g) a globally hyperbolic space-time. The deformation argument of Fulling, Narcowich and Wald [FNW] is based on two facts.

The first fact is the so-called *time slice property* : if $U \subset M$ is a neighborhood of a Cauchy surface Σ, then for any $u \in C_0^\infty(M)$ there exists $v \in C_0^\infty(U)$ such that $u - v \in PC_0^\infty(M)$. In other words

$$C_0^\infty(M)/PC_0^\infty(M) = C_0^\infty(U)/PC_0^\infty(M).$$

This implies that a pair of distributions $\Lambda_\pm \in C_0^\infty(U\times U)$ satisfying :

$$\begin{aligned} &P\circ\Lambda_\pm = \Lambda_\pm\circ P = 0,\\ &\Lambda_+ - \Lambda_- = -{\rm i}E \text{ on } U\times U,\\ &\Lambda_\pm \geq 0 \text{ on } C_0^\infty(U)\end{aligned}$$

generate a quasi-free state on M.

The second fact is *Hörmander's propagation of singularities theorem* (Thm. 9.2) : If $\Lambda_\pm$ satisfy (Had) (or $(genHad)$) over $U\times U$, and $P\circ\Lambda_\pm = \Lambda_\pm\circ P = 0$, then $\Lambda_\pm$ satisfy (Had) or $(genHad)$ globally.

The conclusion of these two facts is that if g_1, g_2 are two Lorentzian metrics such that (M, g_i) is globally hyperbolic, have a common Cauchy surface Σ and coincide in a neighborhood of Σ, then a Hadamard state for the Klein-Gordon field on (M, g_1) generates a Hadamard state for the Klein-Gordon field on (M, g_2).

One argues then as follows : let us fix a Cauchy surface Σ for (M, g) and identify (M, g) with $(\mathbb{R}\times\Sigma, -c^2(t,x)dt^2 + h_{ij}(t,x)dx^i dx^j)$. We set $\Sigma_t = \{t\}\times\Sigma$. We fix a real function $r \in C^\infty(M)$ and consider $P = -\nabla^a\nabla_a + r(x)$ — the associated Klein-Gordon operator. One chooses an ultra-static metric

$$g_{\rm us} = -dt^2 + h_{jk,{\rm us}}({\rm x})d{\rm x}^j d{\rm x}^k, \quad r_{\rm us}(x) = m^2 > 0,$$

and an interpolating metric $g_{\rm int} = -c^2_{\rm int}(t,x)dt^2 + h_{jk,{\rm int}}(x)d{\rm x}^j d{\rm x}^k$, and real function $r_{\rm int} \in C^\infty(M)$ such that $(g_{\rm int}, r_{\rm int}) = (g, r)$ near Σ_T, $(g_{\rm int}, r_{\rm int}) = (g_{\rm us}, m^2)$ Σ_{-T}.

The vacuum state $\omega^{\rm vac}$ for $(M, g_{\rm us})$ is Hadamard for $P_{\rm us}$, hence generates a Hadamard state for $P_{\rm int}$, which itself generates a Hadamard state ω for P.

Using the Cauchy evolution operator from Σ_{-T} to Σ_T, one sees that ω is pure, since $\omega^{\rm vac}$ is pure.

10.3. **Construction of Hadamard states by pseudodifferential calculus.** Let us now briefly describe another construction given in a joint work with Michal Wrochna [GW1]. It relies on the choice of a Cauchy surface Σ and on the global pseudodifferential calculus on Σ.

We identify M with $\mathbb{R}\times\Sigma$, with the split metric $g = -c^2(t,x)dt^2 + h_{ij}(t,x)dx^i dx^j$, and we set $\Sigma_s := \{s\}\times\Sigma \subset M$. For simplicity we will assume that Σ is either equal to $\mathbb{R}^d$ or to a compact manifolds, but much more general situations can be treated as well.

We denote by $\Psi^m(\Sigma)$ the space of (uniform) pseudodifferential operators of order m on Σ, corresponding to quantization of symbols in $S^m_{1,0}(T^*\Sigma)$, and by $\Psi_{\rm ph}(\Sigma)$ the subspace of pseudodifferential operators with poly-homogeneous symbols. We set

$$\Psi^\infty(\Sigma) = \bigcup_{m\in\mathbb{R}} \Psi^m(\Sigma),\ \ \Psi^{-\infty}(\Sigma) = \bigcap_{m\in\mathbb{R}} \Psi^m(\Sigma).$$

We denote by $H^s(\Sigma)$ the Sobolev space of order s on Σ and

$$H^\infty(\Sigma) = \bigcap_{s\in\mathbb{R}} H^s(\Sigma),\ \ H^{-\infty}(\Sigma) = \bigcup_{s\in\mathbb{R}} H^s(\Sigma).$$

We use the third version of the phase space, namely $(C_0^\infty(\Sigma)\otimes\mathbb{C}^2, q)$, where we recall that $q = {\rm i}\sigma_\Sigma$. We embed $C_0^\infty(\Sigma)\otimes\mathbb{C}^2$ into $\mathcal{D}'(\Sigma)\otimes\mathbb{C}^2$ using the natural scalar product on $C_0^\infty(\Sigma)\otimes\mathbb{C}^2$, i.e. we identify sesquilinear forms with operators.

Quasi-free states are now defined by a pair of covariances $\lambda_\pm$ on $C_0^\infty(\Sigma)\otimes\mathbb{C}^2$, and the relationship with the space-time covariances $\Lambda_\pm$ is :

$$\Lambda_\pm = (\rho\circ E)^*\circ\lambda_\pm\circ(\rho\circ E).$$

It is natural to restrict attention to states with covariances $\lambda_\pm \in \Psi^\infty(\Sigma)\otimes M(\mathbb{C}^2)$. It can be shown that if a state has pseudodifferential covariances on Σ_s for some s it has pseudodifferential covariances on Σ_s for any s.

The most important part is to characterize the Hadamard condition in terms of $\lambda_\pm$, which relies on the construction of a parametrix for the Cauchy problem on Σ, see Prop. 10.3 below.

10.3.1. *The model Klein-Gordon equation.* By a change of coordinates and conjugation with a convenient weight, one can reduces oneself to the equation :

$$\partial_t^2 u + a(t,x,\partial_x)u = 0,$$

where $a(t,x,\partial_x)$ is a second order, elliptic selfadjoint operator on $L^2(\Sigma)$.

If $\Sigma = \mathbb{R}^d$ a natural hypothesis (which if needed can be rephrased in terms of the original metric g) is that :

$$a(t,x,\partial_x) = -\sum_{ij} a_{jk}(t,x)\partial_{x^j}\partial_{x^k} + \sum_{a_j}(t,x)\partial_{x^j} + r(t,x),$$

where

$$C^{-1}\xi^2 \leq a_{jk}(t,x)\xi_j\xi_k \leq C\xi^2,$$
$$|\partial_t^m\partial_x^\alpha a_{jk}|,\ |\partial_t^m\partial_x^\alpha a_j],\ \partial_t^m\partial_x^\alpha r \text{ bounded locally uniformly in } t,$$

an assumption of course related to the uniform pdo calculus on Σ. Let us set for $s \in \mathbb{R}$ $\rho_s u := (u\restriction_{\Sigma_s}, \mathrm{i}^{-1}\partial_t u\restriction_{\Sigma_s})$ and U_s the solution of the Cauchy problem on Σ_s, i.e.

$$(\partial_t^2 + a(t))U_s = 0, \rho_s \circ U_s = \mathbb{1}.$$

10.3.2. *Parametrices for the Cauchy problem.* Let $\mathbb{R} \ni t \mapsto b(t)$ is a map with values in linear operators on $L^2(\Sigma)$ with $\mathrm{Dom} b(t) = H^1(\Sigma)$, $b(t) - b^*(t)$ bounded, and $\mathbb{R} \ni t \mapsto b(t)$ be norm continuous with values in $B(H^1(\Sigma), L^2(\Sigma))$. We denote by $\mathrm{Texp}(\mathrm{i}\int_s^t b(\sigma)d\sigma)$ the strongly continuous group with generator $b(t)$. A routine computation shows that

$$(\partial_t^2 + a(t))\mathrm{Texp}(\mathrm{i}\int_s^t b(\sigma)d\sigma) = 0$$

if and only if $b(t)$ solves the following Riccati equation :

$$\mathrm{i}\partial_t b(t) - b^2(t) + a(t) = 0. \tag{10.2}$$

This equation can be solved modulo $C^\infty(\mathbb{R}, \Psi^{-\infty}(\Sigma))$ by symbolic calculus, which amounts to solving transport equations.

Theorem 10.1. *There exists $b(t) \in C^\infty(\mathbb{R}, \Psi^1(\Sigma))$, unique modulo $C^\infty(\mathbb{R}, \Psi^{-\infty}(\Sigma))$ such that*

i) $b(t) = \epsilon(t) + C^\infty(\mathbb{R}, \Psi^0(\Sigma))$,

ii) $(b(t) + b^*(t))^{-1} = \epsilon(t)^{-\frac{1}{2}}(\mathbb{1} + r_{-1}(t))\epsilon(t)^{-\frac{1}{2}},\ r_{-1}(t) \in C^\infty(\mathbb{R}, \Psi^{-1}(\Sigma))$,

iii) $(b(t) + b^*(t))^{-1} \geq c(t)\epsilon(t)^{-1}$, *for some* $c(t) > 0$

iv) $\mathrm{i}\partial_t b - b^2 + a = r_{-\infty} \in C^\infty(\mathbb{R}, \Psi^{-\infty}(\Sigma))$.

Note that if $b^+(t) := b(t)$ solves (10.2), so does $b^-()t := -b^*(t)$. Setting $u^\pm(t,s) = \mathrm{Texpi}\int_s^t b^\pm(\sigma)d\sigma$, we obtain the following result.

Theorem 10.2. *Set*

$$r_s^{0\pm} := \mp(b^+(s) - b^-(s))^{-1}b^\mp(s) \in \Psi^0(\Sigma),$$
$$r_s^{1\pm} := \pm(b^+(s) - b^-(s))^{-1} \in \Psi^{-1}(\Sigma),$$
$$r_s^\pm f := r^{0\pm}f^0 + r^{1\pm}f^1,\ f = (f^0, f^1) \in H^\infty(\Sigma) \otimes \mathbb{C}^2.$$

Then

$$U_s = u^+(\cdot, s)r_s^+ + u^-(\cdot, s)r_s^- + C^\infty(\mathbb{R}, \Psi^{-\infty}(\Sigma)).$$

10.3.3. *Pure Hadamard states.* The following proposition summarizes conditions implying that a pair of operators $\lambda_s^\pm$ are the Cauchy surface covariances (at time s) of a (pure) Hadamard state.

Proposition 10.3. *Let $\lambda_s^\pm : H^\infty(\Sigma)\otimes\mathbb{C}^2 \to H^\infty(\Sigma)\otimes\mathbb{C}^2$ be continuous. Then $\lambda_s^\pm$ are the Cauchy surface covariances of a Hadamard state ω if :*

$$\begin{array}{rl} i) & \lambda_s^{\pm *} = \lambda_s^\pm, \lambda^\pm \geq 0,\\ ii) & \lambda_s^+ - \lambda_s^- = q,\\ iii) & f\in H^{-\infty}(\Sigma)\otimes\mathbb{C}^2 \cap \mathrm{Ker}\lambda^\mp \ \Rightarrow \ \mathrm{WF}(U_s f)\subset N^\pm. \end{array}$$

If additionally $c_s^\pm := \pm \mathrm{i} q^{-1}\circ\lambda_s^\pm$ are projections, *then ω is* pure.

Note that if $f\in H^{-\infty}(\Sigma)\otimes\mathbb{C}^2$ and $r_s^\mp f = 0$, then $\mathrm{WF}U_s f\subset N^\pm$. This allows easily to construct a pure Hadamard state associated to the asymptotic solution $b(t)$ of (10.2).

In fact if we set :

$$T_s(b) = (b(s)+b^*(s))^{-\frac{1}{2}}\begin{pmatrix} b^*(s) & 1\!\!1\\ b(s) & 1\!\!1\end{pmatrix},$$

we note that

$$q = \begin{pmatrix} 0 & 1\!\!1\\ 1\!\!1 & 0\end{pmatrix} = T_s(b)^*\begin{pmatrix} 1\!\!1 & 0\\ 0 & 1\end{pmatrix} T_s(b).$$

It follows that

$$\lambda^\pm(s) := T_s(b)^*\pi^\pm T_s(b),\ \pi^+ = \begin{pmatrix} 1\!\!1 & 0\\ 0 & 0\end{pmatrix},\ \pi^- = \begin{pmatrix} 0 & 0\\ 0 & 1\end{pmatrix},$$

are the Cauchy surface covariances of a pure Hadamard state.

Remark 10.4. *One can show that if the Cauchy surface covariances of a state ω are pseudodifferential at some time s, the same is true at any other time s'.*

Moreover one can show that any *pure Hadamard state with pseudodifferential Cauchy surface covariances is of the form above, for some $t\mapsto b(t)$ as in Thm. 10.1*

The above construction of Hadamard states by pseudodifferential calculus can be generalized to more delicate situations, like *linearized Yang-Mills fields*, where the deformation argument cannot be applied anymore, see [GW2].

10.4. **Construction of Hadamard states by characteristic Cauchy problem.** It is possible to construct Hadamard states by replacing the (space-like) Cauchy surface Σ by some *null* hypersurface C, typically C is chosen to be the *forward lightcone* from some point $p\in M$. Then the interior M_0 of C, when equipped with g is a globally hyperbolic spacetime in its own right. This approach was introduced by Valter Moretti [Mo1], and generalized afterwards to various similar situations, [DMP1, DMP2, DS, Mo2] in order to construct a distinguished Hadamard state on *asymptotically flat* spacetimes, for the conformal wave equation.

In [GW3] we construct a large family of pure Hadamard states on the cone C, using again pseudodifferential calculus.

10.4.1. *The geometric framework.* Let (M, g) a globally hyperbolic spacetime, $p \in M$ a distinguished point of M. Let

$$C := \partial J^{+}(p)\backslash\{p\}$$

be the future lightcone from p and

$$M_0 = I^{+}(p) \text{ its interior.}$$

One can show that (M_0, g) is also a globally hyperbolic spacetime. Moreover one can show that :

$$J^{+}(K; M_0) = J^{+}(K; M),\ J^{-}(K; M_0) = J^{-}(K; M) \cap M_0,\ \forall\ K \subset M_0. \tag{10.3}$$

Some global conditions are needed to avoid singularities of C. One assumes that there exists $f \in C^{\infty}(M)$ such that :

(1) $C \subset f^{-1}(\{0\}),\ \nabla_a f \neq 0$ on $C,\ \nabla_a f(p) = 0,\ \nabla_a \nabla_b f(p) = -2g_{ab}(p)$,

(2) the vector field $\nabla^a f$ is complete on C.

Note that since C is a null hypersurface the vector field $\nabla^a f$ is tangent to C.

From this hypothesis it is easy to construct coordinates (f, s, θ) near C, with $f, s \in \mathbb{R}$, $\theta \in \mathbb{S}^{d-1}$ such that $C \subset \{f = 0\}$ and

$$g\restriction_C = -2df ds + h(s, \theta)d\theta^2, \tag{10.4}$$

where $h(s, \theta)d\theta^2$ is a Riemannian metric on $\mathbb{S}^{d-1}$.

Such choice of coordinates allows one to identify C with $\tilde{C} := \mathbb{R} \times \mathbb{S}^{d-1}$. A natural space of smooth functions on $\tilde{C}$ is then provided by $H^{\infty}(\tilde{C})$ — the intersection of Sobolev spaces of all orders, defined using the round metric $m(\theta)d\theta^2$ on $\mathbb{S}^{d-1}$.

10.4.2. *Bulk to boundary correspondence.* Let us consider the restriction P_0 of the Klein-Gordon operator P to $C^{\infty}(M_0)$, and $E_{0\pm}$ its advanced/retarded Green's functions. From (10.3), one obtains $E_{0\pm} = E_{\pm}\restriction_{M_0\times M_0}$, hence :

$$E_0 = E\restriction_{M_0\times M_0}\ .$$

This implies that any solution $\phi_0 \in \mathrm{Sol}_{\mathrm{sc}}(P_0)$ uniquely extends to $\phi \in \mathrm{Sol}_{\mathrm{sc}}(P)$. In particular its trace $\phi_0\restriction_C$ is well defined.

It is convenient to introduce the coordinates (s, θ) on C, and to set :

$$\begin{aligned} \rho:\ \ & \mathrm{Sol}_{\mathrm{sc}}(P_0) \to C^{\infty}(\mathbb{R} \times \mathbb{S}^{d-1}) \\ & \phi \mapsto \beta^{-1}(s, \theta)\phi\restriction_C (s, \theta), \end{aligned}$$

for

$$\beta(s, \theta) := |m|^{\frac{1}{4}}(\theta)|h|^{-\frac{1}{4}}(s, \theta),$$

where $h(s, \theta)d\theta^2$ is defined in (10.4) and $m(\theta)d\theta^2$ is the round metric on $\mathbb{S}^{d-1}$.

We equip $H^{\infty}(\tilde{C})$ with the symplectic form :

$$\overline{g}_1\sigma_C g_2 := \int_{\mathbb{R}\times\mathbb{S}^{d-1}} (\partial_s\overline{g}_1 g_2 - \overline{g}_1\partial_s g_2)|m|^{\frac{1}{2}}(\theta)dsd\theta,\ g_1, g_2 \in \mathcal{H}(\tilde{C}). \tag{10.5}$$

Introducing the *charge* $q := \mathrm{i}\sigma_C$ we have :

$$\overline{g}_1 q g_2 = 2(g_1|D_s g_2)_{L^2(\tilde{C})},\ g_1, g_2 \in \mathcal{H}(\tilde{C}), \tag{10.6}$$

where $D_s = \mathrm{i}^{-1}\partial_s$ is selfadjoint on $L^2(\tilde{C})$ on its natural domain. Clearly $(H^\infty(\tilde{C}), \sigma_C)$ is a complex symplectic space.

One can show the following result (the second statement follows from Stokes theorem), which summarizes the *bulk to boundary correspondence* :

Proposition 10.5. (1) *ρ maps $\mathrm{Sol}_{\rm sc}(P_0)$ into $\mathcal{H}(\tilde{C})$;*

(2) *$\rho : (\mathrm{Sol}_{\rm sc}(P_0), \sigma) \to (\mathcal{H}(\tilde{C}), \sigma_C)$ is a monomorphism, i.e. :*

$$\overline{\rho\phi}_1 \sigma_C \rho\phi_2 = \overline{\phi}_1 \sigma \phi_2, \ \forall \phi_1, \phi_2 \in \mathrm{Sol}_{\rm sc}(P_0).$$

10.4.3. *Hadamard states on the cone.* From Prop. 10.5, we see that any quasi-free state ω_C on $\mathrm{CCR}(H^\infty(\tilde{C}), \sigma_C)$ generates a quasi-free state ω_0 on $\mathrm{CCR}(C_0^\infty(M_0)/PC_0^\infty(M_0), E_0)$. The task is now to give conditions on ω_C implying that ω_0 is Hadamard.

Let us denote by $x = (r, s, y)$ the coordinates (f, s, θ) near C and by $\xi = (\rho, \sigma\eta)$ the dual coordinates. The complex covariances of ω_C are denoted by $\lambda^\pm \in \mathcal{D}'(\tilde{C} \times \tilde{C})$. The associated covariances $\Lambda^\pm$ of ω_0 are then :

$$\Lambda^\pm := (\rho \circ E_0)^* \circ \lambda^\pm \circ (\rho \circ E_0).$$

One can show the following result.

Theorem 10.6. *Assume that $\lambda^\pm : H^\infty(\tilde{C}) \to H^\infty(\tilde{C})$ and ${}_{\tilde{C}}\mathrm{WF}(\lambda^\pm)' = \mathrm{WF}(\lambda^\pm)'_{\tilde{C}} = \emptyset$ Then if :*

$$\begin{aligned} &i)\ \mathrm{WF}(\lambda^\pm)' \cap \{(Y_1, Y_2) : \pm\sigma_1 < 0 \ \mathit{or} \ \pm\sigma_2 < 0\} = \emptyset, \\ &ii)\ \mathrm{WF}(\lambda^\pm)' \cap \{(Y_1, Y_2) : \pm\sigma_1 > 0 \ \mathit{and} \ \pm\sigma_2 > 0\} \subset \Delta. \end{aligned}$$

$\Lambda^\pm$ satisfy (Had).

A state on $\mathrm{CCR}(H^\infty(\tilde{C}), \sigma_C)$ satisfying the assumptions of Thm. 10.6 will be called a *Hadamard state on the cone.*

10.4.4. *Hadamard states on the cone and pseudodifferential calculus.* Recall that q defined in (10.6) equals $2D_s$, whose resolvent $(2D_s - z)^{-1}$ is not an elliptic pseudodifferential operator on $\tilde{C}$, for the usual calculus. However it belongs to a larger *bi-homogeneous class* $\Psi^{p_1,p_2}(\tilde{C})$, which can be loosely defined as $\Psi^{p_1}(\mathbb{R}) \otimes \Psi^{p_2}(\mathbb{S}^{d-1})$.

It is then possible to construct Hadamard states on the cone by mimicking the arguments in Subsect. 10.3. Note that no construction of a parametrix for the characteristic Cauchy problem on $\tilde{C}$ is necessary, since the Hadamard condition on the cone is rather explicit.

10.4.5. *Purity inside the cone.* A natural issue with this construction is whether a pure state on the cone generates a pure state inside. This is not a priori obvious, since the map ρ is not surjective. Nevertheless it is shown in [GW3] that purity is preserved, using the results of Hörmander [Hö] on the characteristic Cauchy problem. This is the only place where the solvability of the characteristic Cauchy problem is important.

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