Reading Note on Quantum Field Theory in Curved Spacetime

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Abstract

In this note we consider the quantum field theory with curved spacetime background of 3+1 dimensions, following the approach of R. M. Wald [1].

Contents

1 Introduction

The topic of quantum field theory in curved spacetime refers to the theories of quantum fields living in classical spacetime background, namely, a manifold with Lorentzian signature. All fields are treated to be quantized except that the spacetime metric remains a classical object. For most times the metric will be treated as fixed, except when we consider back reactions.

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The field theories built in this manner have finite range of validity. For instance, we expect that it will break down when the energy scale is around Planck mass. However, they are able to cover a variety of phenomena including cosmological particle generation, Hawking radiation, etc.

To generalize QFT from flat spacetime to curved ones needs us to reconsider a number of basic settings in the former case, in which many concepts are introduced with a strong dependence of Poincaré symmetry.

2 Quantum Mechanics and QFT in Flat Spacetime

In this section we will develop a formalism of quantizing a classical system which can be applied directly to field theories with curved spacetime. This formalism differs significantly from the the way one usually encounter in quantum field theory in Minkowski spacetime. Therefore we will develop it step by step, and make comparisons with conventional approach at each corner.

2.1 Classical mechanics

We begin with a classical system with finite degrees of freedom. Such a system can be described as follows. Let $q_1, \cdots, q_n$ be the generalized coordinates of the system and $p_1, \cdots, p_n$ their conjugate momenta. Then $(q_1, \cdots q_n; p_1, \cdots, p_n)$ span the phase space of the system. The dynamics of the system is given by the Hamiltonian $H = H(q_i, p_i)$, which is a function defined over the phase space. The time evolution of the system is governed by the Hamilton's equations,

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i}, \qquad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}. \tag{1}$$

Equivalently, we can define $y = (q_1, \cdots, q_n; p_1, \cdots, p_n)$ and the $2n \times 2n$ antisymmetric matrix

$$\Omega^{ab} = \begin{pmatrix} 0_{n\times n} & I_{n\times n} \\ -I_{n\times n} & 0_{n\times n} \end{pmatrix}, \tag{2}$$

and rewrite equations (2) as

$$\frac{\mathrm{d}y^a}{\mathrm{d}t} = \Omega^{ab}\frac{\partial H}{\partial y^b}. \tag{3}$$

Such a system can be generalized: We can take the phase space of the system to be a $2n$-dimensional manifold $\mathscr{M}$ with a symplectic form Ω_{ab}. That is, Ω_{ab} is a nondegenerate, closed 2-form, satisfying $\Omega_{ab} = -\Omega_{ba}$ and $\nabla_{[a}\Omega_{bc]} = 0$. Nondegeneracy implies that Ω_{ab} has a unique inverse Ω^{ab} such that $\Omega^{ab}\Omega_{bc} = \delta^a{}_c$. The Hamiltonian, then, is still given by a function $H : \mathscr{M} \to \mathbb{R}$. Furthermore, we can define the Hamiltonian vector field on $\mathscr{M}$, to be $h^a = \Omega^{ab}\nabla_b H$. Then, the law of time evolution, namely the Hamilton's equation, is simply the statement that the dynamical evolution of the system is given by the integral curves of h^a.

This generalized description coincides with the original one, at least locally. In fact, the phase space defined as the span of (q_i, p_i) can be regarded as a cotangent bundle, $\mathscr{M} = T_*(\mathscr{Q})$, with $\mathscr{Q}$ the configuration space spanned by coordinates q_i. The symplectic form Ω_{ab} is given by $\Omega_{ab} = 2(\nabla_{[a}p_i)(\nabla_{b]}q_i)$, or in the language of differential forms:

$$\Omega = \mathrm{d}p_i \wedge \mathrm{d}q_i. \tag{4}$$

Conversely, from a phase space defined as a symplectic manifold $(\mathscr{M},\Omega)$, Darboux theorem tells us that one can always find a local coordinates on a neighborhood of $\mathscr{M}$ such that the symplectic form Ω in this coordinate system takes the form of (4). The advantage of using the language of symplectic manifold is that it is independent of choice of canonical variables.

In a classical system, observables can be defined to be C^∞ functions on $\mathscr{M}$. Obviously, $C^\infty(\mathscr{M})$ is a linear space. With Ω^{ab}, we can define a product on $C^\infty(\mathscr{M})$ which we call Poisson bracket. For any $f,g\in C^\infty(\mathscr{M})$, we define their Poisson bracket, $\{f,g\}$, to be

$$\{f,g\}=\Omega^{ab}(\nabla_a f)(\nabla_b g). \tag{5}$$

It is easy to check that $\{f,g\}\in C^\infty(\mathscr{M})$, and that the bracket is antisymmetric, and satisfies the Jacobi identity.

Canonical variables themselves, in particular, are observables. Their Poisson bracket can be found with the expression of Ω, (4), to be

$$\{q_i,q_j\}=\{p_i,p_j\}=0, \qquad \{q_i,p_j\}=\delta_{ij}. \tag{6}$$

From now on, we will restrict ourselves to linear system, which satisfies the following two conditions: 1) The phase space $\mathscr{M}$ is given by the cotangent bundle of the configuration space $\mathscr{Q}$, $\mathscr{M}=T_*(\mathscr{Q})$, where $\mathscr{Q}$ is set to be a linear space; 2) Hamiltonian function $H:\mathscr{M}\to\mathbb{R}$ is quadratic in coordinates of $\mathscr{M}$.

Let's see what consequences do these two linear conditions lead to. Firstly, the linear structure of $\mathscr{Q}$ naturally makes $\mathscr{M}$ also a linear space, on which a global coordinate system (q_i,p_i) can be assigned. The symplectic form Ω_{ab}, then, becomes a bilinear map $\Omega:\mathscr{M}\times\mathscr{M}\to\mathbb{R}$. $\forall y_1,y_2\in\mathscr{M}$ with $y_1=(q_{1i},p_{1i})$, $y_2=(q_{2i},p_{2i})$,

$$\Omega(y_1,y_2)=p_{1i}q_{2i}-p_{2i}q_{1i}. \tag{7}$$

That is, $\mathscr{M}$ becomes a symplectic (linear) space. In this case, a crucial observation is that coordinates on $\mathscr{M}$ can be represented in terms of Ω. For instance, if we take $y=(q_i,p_i)$ with $q_i=(1,0,\cdots,0)$ and $p_i=(0,\cdots,0)$, then $\Omega(y,\cdot)$, as a linear map on $\mathscr{M}$, simply picks out the minus "p_1"-component of the vector on which it acts. Similarly, for $q_i=(0,\cdots,0)$ and $p_i=(1,0,\cdots,0)$, $\Omega(y,\cdot)$ picks out the q_1-component. In general, when y runs over $\mathscr{M}$, $\Omega_{y,\cdots}$ gives all possible linear combinations of all components of the vector on which it acts. Therefore one can rewrite expressions involving canonical variables in terms of $\Omega(y,\cdots)$. In particular, the Poisson bracket of canonical variables can be rewritten as

$$\big\{\Omega(y_1,\cdot),\Omega(y_2,\cdot)\big\}=-\Omega(y_1,y_2). \tag{8}$$

The advantage of using this somewhat sophisticated notation is, again, the independence of choice of coordinates.

Now let's consider the solutions of Hamilton's equation. Since the solution is uniquely determined once we assign a point $y\in\mathscr{M}$ as the initial condition at time $t=0$, we can naturally identify the space $\mathscr{S}$ of all solutions of Hamilton's equation with $\mathscr{M}$. By the linearity condition 2), $\mathscr{S}$ is also a linear space. Furthermore, we can carry the symplectic structure of $\mathscr{M}$ into $\mathscr{S}$. To see this, let us write the Hamiltonian as follows without loss of generality,

$$H(t;y)=\frac{1}{2}K_{ij}(t)y^iy^j, \qquad \forall y\in\mathscr{M}, \tag{9}$$

where $K_{\mu\nu}$ is a symmetric matrix. Then the Hamilton's equation becomes:

$$\frac{\mathrm{d}y^i}{\mathrm{d}t} = \Omega^{ij} K_{jk} y^k. \tag{10}$$

Suppose $y_1(y)$ and $y_2(t)$ are two solutions, we define their symplectic product $s(t)$, by

$$s(t) = \Omega(y_1(t), y_2(y)) = \Omega_{ij} y_1^i y_2^j. \tag{11}$$

It is straightforward to show that $s(t)$ is actually independent of t,

$$\begin{aligned}\frac{\mathrm{d}s}{\mathrm{d}t} &= \Omega_{ij}\Big(\frac{\mathrm{d}y_1^i}{\mathrm{d}t} y_2^j + y_1^i \frac{\mathrm{d}y_2^j}{\mathrm{d}t}\Big) = \Omega_{ij}\big(\Omega^{im} K_{mn} y_1^n y_2^j + \Omega^{jm} K_{mn} y_2^n y_1^i\big)\\ &= -K_{jn} y_1^n y_2^j + K_{in} y_1^i y_2^n = 0.\end{aligned}$$

Therefore, this symplectic product of solutions gives a symplectic structure of $\mathscr{S}$.

2.2 Quantum mechanics

In classical mechanics the state of a system is represented by a point in phase space. Its dynamical evolution is dictated by the canonical transformation generated by Hamiltonian function. Observables are represented by functions on phase space. In quantum mechanics, one use vectors in state space to describe the system, and the unitary transformation generated by Hamiltonian operator to describe the time evolution. Observables are represented by self-adjoint operators on the state space.

The procedure of quantization, is to seek a correspondence between these two pictures. The kernel of this correspondence is the symplectic structure, which is described by Poisson bracket on classical side and by commutator on quantum side. Therefore, quantizing a classical system amounts to find an appropriate state space and associated self-adjoint operators served as observables, such that there exists a map, which we denote by " $\widehat{\ }$ ", between classical observables and quantum self-adjoint operators, $\widehat{\ } : f \to \widehat{f}$, such that

$$[\widehat{f}, \widehat{g}] = \mathrm{i}\widehat{\{f, g\}}. \tag{12}$$

Unfortunately, this is generally impossible. That is, these exists no such a map which send all classical observables to quantum self-adjoint operators in a manner consistent with Schrödinger's quantization procedure (See, e.g., [2]). Nevertheless, it is possible to find a map which send canonical variables, together with observable at most linear in canonical variables, into operators, such that,

$$[\widehat{q}_i, \widehat{q}_j] = [\widehat{p}_i, \widehat{p}_j] = 0, \qquad [\widehat{q}_i, \widehat{p}_j] = \mathrm{i}\widehat{\{q_i, p_j\}} = \mathrm{i}\delta_{ij} I. \tag{13}$$

Now let us restrict ourselves to linear theory. According to the last subsection, we would generalize the commutator above in the following coordinate-independent manner:

$$\big[\widehat{\Omega}(y_1, \cdot), \widehat{\Omega}(y_2, \cdot)\big] = -\mathrm{i}\Omega(y_1, y_2) I, \qquad \forall y_1, y_2 \in \mathscr{M}. \tag{14}$$

However for technical reasons (the self-adjoint operators appearing here may be unbounded and commutators cannot be well-defined), we should consider the unitary operators $W(y) \equiv e^{\mathrm{i}\Omega(y,\cdot)}$ instead. Then the condition imposed on quantized operator $\widehat{W}$ are as follows:

$$1) \qquad \widehat{W}(y_1)\widehat{W}(y_2) = e^{\mathrm{i}\Omega(y_1,y_2)/2}\widehat{W}(y_1 + y_2); \tag{15}$$

$$2) \qquad \widehat{W}^\dagger(y) = \widehat{W}(-y). \tag{16}$$

There two conditions are called Weyl relations. Then the quantization is a procedure of seeking for a state space $\mathscr{F}$ and observables $\widehat{f}_i$ on it, such that there exists a map $\widehat{\ }: f_i \to \widehat{f}_i$ satisfying Weyl relations. The state space $\mathscr{F}$ together with observables $\widehat{f}_i$ obtained in this way is called a representation of Weyl relations.

There is a theorem showing that Weyl relations bring strong constraint to the choice of the quantum state space of a system of finite degrees of freedom. To state this theorem, we note in advance that a representation $(\mathscr{F}, \widehat{W})$ of Weyl relations is said to be irreducible, if for given $\Psi \in \mathscr{F}$, $\{\widehat{W}(y)\Psi | y \in \mathscr{M}\}$ is a dense subset of $\mathscr{F}$. Two representations $(\mathscr{F}_1, \widehat{W}_1)$ and $(\mathscr{F}_2, \widehat{W}_2)$ are said to be unitarily equivalent, if there is a unitary map $U : \mathscr{F}_1 \to \mathscr{F}_2$ such that $\widehat{W}_2(y) = U\widehat{W}_1(y)U^{-1}$ for all y. Then, we have the following:

Theorem. (Stone-von Neumann theorem) *Let* $(\mathscr{M}, \Omega)$ *be finite dimensional symplectic space, let* $(\mathscr{F}_1, \widehat{W}_1(y))$ *and* $(\mathscr{F}_2, \widehat{W}_2(y))$ *be two strongly continuous*[1]*, irreducible representations of Weyl relations. Then* $(\mathscr{F}_1, \widehat{W}_1(y))$ *and* $(\mathscr{F}_2, \widehat{W}_2(y))$ *are unitarity equivalent.*

Note that SvN theorem says nothing about observables other than canonical variables. As mentioned above, observables at most linear in canonical variables can also be unambiguously mapped to self-adjoint operators. In other cases, there is factor ordering ambiguity. Furthermore, the condition of finite dimension of phase space in SvN theorem is crucial, in that when the classical system contains infinitely many degrees of freedom, as happens in field theory, there actually exists an infinite number of unitarily inequivalent irreducible representations of Weyl relations. In Minkowski spacetime, Poincaré symmetry picks out a preferred representation among others. But in curved spacetime, there is in general no way to select out a preferred representation. We will discuss this topic further in the next section.

As the final remark of this subsection, we note that in conventional Schrödinger procedure of quantization of a 3 dimensional system, one takes the state space to be $L^2(\mathbb{R}^3)$, and $\widehat{q}_\mu$ is defined to be multiplying the state function by q_μ, and $\widehat{p}_\mu$ is defined to be $-\mathrm{i}\partial/\partial q_\mu$. It can be shown that the result is an irreducible representation of Weyl relations. SvN theorem then guarantees that any other irreducible construction of quantum theory of this system is unitarily equivalent to the one obtained by Schrödinger's procedure.

2.3 Harmonic oscillators

As a warming-up exercise, let's consider a system of n uncoupled harmonic oscillators. For each of them, the Lagrangian and Hamiltonian function are given by

$$L = \tfrac{1}{2}p^2 - \tfrac{1}{2}\omega^2 q^2, \qquad H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2 q^2, \tag{17}$$

[1]Strong continuity means the continuity under the strong operator topology.

respectively. We can following Schrödinger's procedure, taking the state space to be $\mathscr{F} = L^2(\mathbb{R})$, and taking $q \to \widehat{q} = q\times$, $p \to \widehat{p} = -\mathrm{i}\partial/\partial q$. We further define

$$a = \sqrt{\frac{\omega}{2}}q + \mathrm{i}\sqrt{\frac{1}{2\omega}}p. \tag{18}$$

Then the Hamiltonian operator can be written as $H = \omega(a^\dagger a + \frac{1}{2}I)$. The state space can constructed from vacuum state Ψ_0 satisfying $a\Psi_0 = 0$, by applying $a^\dagger$ any times: $\Psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\Psi_0$. Then the state space $\mathscr{F}$ is spanned by $\{\Psi_i\}_{i=0}^\infty$.

For n uncoupled harmonic oscillators with frequencies ω_i $(i = 1, \cdots, n)$, the state space can be taken to be the tensor product of state spaces of individual oscillators,

$$\mathscr{F} = \bigotimes_{i=1}^n \mathscr{F}_i. \tag{19}$$

On the other hand, we can reconstruct the quantum theory along a new way which can be directly generalized to the case of field theories. We begin with the symplectic space $(\mathscr{S}, \Omega)$ of solutions of classical equation of motion, introduced in Subsection 2.1. The first step of our construction is to complexify $\mathscr{S}$ into a complex linear space $\mathscr{S}^\mathbb{C}$, and introduce a bilinear map $(\cdot,\cdot) : \mathscr{S}^\mathbb{C} \times \mathscr{S}^\mathbb{C} \to \mathbb{C}$, by

$$(y_1, y_2) = -\mathrm{i}\Omega(\bar{y}_1, y_2), \qquad \forall y_1, y_2 \in \mathscr{S}^\mathbb{C}. \tag{20}$$

Note that this bilinear map fails to be a inner product on $\mathscr{S}^\mathbb{C}$ since it is not positively definite. However, we notice that when restricted to the space $\mathscr{H}$ spanned by solutions of positive frequency, namely solutions of the form $q_i(t) = \alpha_i e^{-\mathrm{i}\omega_i t}$, it can be shown (show it!) that this bilinear map is positively definite, and turns into an inner product. It follows that $\mathscr{H}$ is a n-complex dimensional Hilbert space. The normalized solutions ξ_i $(i = 1, \cdots, n)$ with $(\xi_i, \xi_i) = 1$ then form an orthonormal basis of $\mathscr{H}$.

Then, we take the state space $\mathscr{F}$ of the system to be the symmetric Fock space of $\mathscr{H}$, namely $\mathscr{F} = F_S(\mathscr{H})$, or more elaborately,

$$F_S(H) = \bigoplus_{n=1}^\infty \Big(\otimes_S^n \mathscr{H} \Big), \tag{21}$$

with $\otimes_S^n$ representing the symmetric tensor product of n copies, while $\otimes_S^0 \mathscr{H} \equiv \mathbb{C}$. Then, a state $\Psi \in \mathscr{F}$ can be represented as

$$\Psi = (\psi, \psi^{a_1}, \psi^{a_1 a_2}, \cdots, \psi^{a_1 \cdots a_n}, \cdots), \tag{22}$$

where the indices of each ψ are totally symmetric. In such a Fock space $F_S(\mathscr{H})$, one can define the annihilation operator $a(\bar{\xi})$ associated a vector $\bar{\xi}^a \in \bar{\mathscr{H}}$, by

$$a(\bar{\xi})\Psi = (\bar{\xi}_a \psi^a, \sqrt{2}\bar{\xi}_a \psi^{a a_1}, \sqrt{3}\bar{\sigma}_a \psi^{a a_1 a_2}, \cdots), \tag{23}$$

where the contraction of indices means the "inner product" on $\mathscr{S}^\mathbb{C}$. Similarly, the creation operator associated with $\xi \in \mathscr{H}$ is defined by

$$a^\dagger(\xi)\Psi = (0, \psi\xi^{a_1}, \sqrt{2}\xi^{(a_1}\psi^{a_2)}, \sqrt{3}\xi^{(a_1}\psi^{a_2 a_3)}, \cdots). \tag{24}$$

Annihilation and creation operators defined in such way satisfy the commutation relation,

$$[a(\bar{\xi}), a^\dagger(\eta)] = (\xi, \eta)I. \tag{25}$$

Now we take a_i to be the annihilation operator associated with $\bar{\xi}_i$, and define the Heisenberg operators associated with coordinate and momenta to be

$$q_{i\mathrm{H}}(t) = \xi_i(t)a + \bar{\xi}_i(t)a_i^\dagger, \qquad p_{i\mathrm{H}}(t) = \frac{\mathrm{d}q_{i\mathrm{H}}}{\mathrm{d}t}. \tag{26}$$

Either by SvN theorem or by direct checking, we know that the quantum theory constructed in this way is unitarily equivalent to the one obtained above by Schrödinger construction.

With slight modification, we can reexpress the Fock space construction in a coordinate-independent manner. It is easy to see that in our case, $\forall y \in \mathscr{S}^{\mathbb{C}}$, there exist a unique $y^+ \in \mathscr{H}$ and a unique $y^- \in \bar{\mathscr{H}}$ such that $y = y^+ + y^-$. It follows directly that there exists a projection operator $K : \mathscr{S}^{\mathbb{C}} \to \mathscr{H}$ projecting a solution to its positive-frequency component. Then, $\forall y \in \mathscr{S}$, the classical variable, represented as $\Omega(y, \cdot)$, corresponds to the following quantum operator in Schrödinger picture:

$$\widehat{\Omega}(y, \cdot) = \mathrm{i}a(\overline{Ky}) - \mathrm{i}a^\dagger(Ky). \tag{27}$$

We can also write down the operators of canonical variables in Heisenberg picture,

$$\widehat{\Omega}_{\mathrm{H}}(y, \cdot) = \mathrm{i}a(\overline{Ky_t}) - \mathrm{i}a^\dagger(Ky_t), \tag{28}$$

where y_t denotes the classical solution which at time t takes the same value as y at $t = 0$.

Next, we generalize the above construction to the case in which the Hamiltonian is time dependent. Now there is no definite meaning to talk about solutions of positive or negative frequency, and thus there is no natural way to select out the space $\mathscr{H}$. But we can make it conversely. In light of the properties of $\mathscr{H}$ defined in above case, now we can take the desired space $\mathscr{H}$ to be anyone satisfying the following three conditions:

1. The bilinear map $(,)$ defined via (20) is positively definite on $\mathscr{H}$;
2. $\mathscr{S}^{\mathbb{C}}$ is spanned by $\mathscr{H}$ and $\bar{\mathscr{H}}$;
3. $\forall y^+ \in \mathscr{H}$ and $\forall y^- \in \bar{\mathscr{H}}$, we have $(y^+, y^-) = 0$.

It follows directly that $\forall y \in \mathscr{S} \subset \mathscr{S}^{\mathbb{C}}$, y can be uniquely decomposed as $y = y^+ + y^-$ with $y^+ \in \mathscr{H}$ and $y^- \in \bar{\mathscr{H}}$, or equivalently, there exists the projection operator $K : \mathscr{S} \to \mathscr{H}$.

Once the space H is chosen, we can still take the quantum state space to be $F_S(\mathscr{H})$, and take the Heisenberg operators of canonical variables to be given by (28).

It is worth noting that the construction above is independent of choice of canonical variable, but depends on the choice of $\mathscr{H}$. We will study this dependence further in the following.

2.4 Quantum fields in Minkowski spacetime

We consider real and noninteracting Klein-Gordon field, with the action given by

$$S = -\frac{1}{2}\int \mathrm{d}^4x \left((\partial_a\phi)(\partial^a\phi) + m^2\phi^2\right). \tag{29}$$

The conventional approach of quantization begins with taking the spacetime to be 3-torus T^3, and expanding the solution of the classical equation of motion $(\partial^2 - m^2)\phi = 0$ in terms of plane waves,

$$\phi(t, \mathbf{x}) = \frac{1}{L^{3/2}} \sum_{\mathbf{k}} \phi_{\mathbf{k}}(t) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \qquad \phi_{\mathbf{k}}(t) = \frac{1}{L^{3/2}} \int \mathrm{d}^3x\, \phi(t, \mathbf{x}) e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{30}$$

The reality of the field, namely $\bar{\phi}(t, \mathbf{x}) = \phi(t, \mathbf{x})$ implies that $\bar{\phi}_{\mathbf{k}} = \phi_{-\mathbf{k}}$. As a result, the Lagrangian can be rewritten in terms of modes, as

$$L = \frac{1}{2} \sum_{\mathbf{k}} \Big(|\dot{\phi}_{\mathbf{k}}|^2 - \omega_{\mathbf{k}}^2 |\phi_{\mathbf{k}}|^2 \Big), \tag{31}$$

with $\omega_{\mathbf{k}} \equiv \mathbf{k}^2 + m^2$, and this is actully a system of infinitely many uncoupled harmonic oscillators.

To quantize this system, we need a quantum state space. Here the tensor product space is not suitable since it is too large, in the sense that it is a reducible representation of Weyl relations. Instead, we will adopt Fock space construction. That is, we pick out the space of positive-frequency solutions $\mathscr{H}$, which is spanned by eigenfunction

$$\psi_{\mathbf{k}}(t, \mathbf{x}) = \frac{1}{\sqrt{2\omega_{\mathbf{k}} L^3}} e^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)}, \tag{32}$$

from the whole solution space $\mathscr{S}$, and define the inner product as was done in (20), to turn $\mathscr{H}$ into a Hilbert space. The following steps are in parallel with that of harmonic oscillators: 1) The quantum state space is given by the symmetric Fock space of $\mathscr{H}$, namely $F_S(\mathscr{H})$. 2) We take $a_{\mathbf{k}}$ to be the annihilation operator associated with $\bar{\psi}_{\mathbf{k}}$, which, together with its Hermite conjugation, satisfies the familiar commutation relations $[a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0$, $[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'} I$. 3) The quantum field operator in Heisenberg picture is

$$\hat{\phi}(t, \mathbf{x}) = \sum_{\mathbf{k}} \Big(\psi_{\mathbf{k}}(t, \mathbf{x}) a_{\mathbf{k}} + \text{h.c.} \Big). \tag{33}$$

Now we would like to reformulate the quantum field theory in Minkowski space-time in a coordinate-independent manner. Taking the 3-dimensional hypersurface Σ_0 of constant time. Then the field $\phi(x)$ together with its conjugate momentum $\pi = \delta S / \delta\dot{\phi} = \dot{\phi}$ on Σ_0 uniquely determines a solution of classical equation of motion. Therefore, the classical phase space is spanned by all possible functions assigned to $\phi(x)$ and $\pi(x)$ on Σ_0. The problem is, then, what class of functions is permissible? The basic requirements on these functions are that they should be well behaved such that the mathematical structures such like symplectic forms can be defined, while this class of functions cannot be too restrictive to reflect local degrees of freedom of fields. For our purpose, it is suitable to take $\phi(x)$ and $\pi(x)$ to be test functions, i.e., smooth functions with compact support. We denote the space of test functions on Σ_0 by $C_0^\infty(\Sigma_0)$. Then, the classical phase space is given by

$$\mathscr{M} = \big\{ (\phi, \pi) | \phi, \pi \in C_0^\infty(\Sigma_0) \big\}. \tag{34}$$

The symplectic product of two points in $\mathscr{M}$ are given by

$$\Omega\big((\phi_1, \pi_1), (\phi_2, \pi_2) \big) = \int_{\Sigma_0} \mathrm{d}^3x\, (\pi_1 \phi_2 - \pi_2 \phi_1), \tag{35}$$

and the Poisson bracket is defined as before:

$$\big\{\Omega\big((\phi_1,\pi_1),\cdot\big),\Omega\big((\phi_2,\pi_2),\cdot\big)\big\}=-\Omega\big((\phi_1,\pi_1),(\phi_2,\pi_2)\big). \tag{36}$$

Note that this expression is already independent of choice of basis in phase space, and thus can be generalized directly to the case of curved spacetime. To send this abstract equation back to our familiar one, we make a particular choice that $(\phi_1,\pi_1)=(0,f_1)$, $(\phi_2,\pi_2)=(f_2,0)$. Then, substitute an arbitrary $(\phi,\pi)\in\Sigma_0$ for the dot in equation above, we get

$$\left\{\int_{\Sigma_0}\mathrm{d}^3x\,f_1\phi\;,\;\int_{\Sigma_0}\mathrm{d}^3x\,f_2\pi\right\}=\int_{\Sigma_0}\mathrm{d}^3x\,f_1f_2. \tag{37}$$

In a familiar but somewhat loose notation, this result can be rewritten as

$$\{\phi(x_1),\pi(x_2)\}=\delta(x_1-x_2). \tag{38}$$

To quantize this classical system with phase space $\mathscr{M}$, we again begin with the solution space $\mathscr{S}$, which can still be identified with $\mathscr{M}$. We complexify $\mathscr{S}$ into $\mathscr{S}^{\mathbb{C}}$, take the subspace of positive frequency solutions $\mathscr{S}^{\mathbb{C}+}$, and define inner product on $\mathscr{S}^{\mathbb{C}+}$ by $(\psi^+,\chi^+)=-\mathrm{i}\Omega(\bar{\psi}^+,\chi^+)$. Then we Cauchy-complete $\mathscr{S}^{\mathbb{C}+}$ under this inner product to turn it into a Hilbert space $\mathscr{H}$. The unique decomposition of solutions into positive and negative frequency parts $\psi=\psi^++\psi^-$ still works, and it gives a projection K from $\mathscr{S}$ onto a dense subset of $\mathscr{H}$. Then, the quantum state space is again given by the symmetric Fock space $F_S(\mathscr{H})$. The quantum operator associated with $\psi\in\mathscr{S}$ is given by

$$\widehat{\Omega}(\psi,\cdot)=\mathrm{i}a(\overline{K\psi})-\mathrm{i}a^\dagger(K\psi). \tag{39}$$

2.5 Particle Interpretation

Now we will consider the question of how the concept of particles arises in field theories, in what sense we call an excited state of quantum fields a particle. In this investigation, the notion of particle detector is important.

Let's consider the simplest case, a real Klein-Gordon field in Minkowski spacetime coupled to a two-state system, whose Hamiltonian is given by

$$H=H_\phi+H_q+H_{\text{int.}}, \tag{40}$$

where $H=\frac{1}{2}\int\mathrm{d}^3x\,\big(\dot{\phi}^2+(\nabla\phi)^2+m^2\phi^2\big)$. For two-state system, let's assume its two energy states to be $|\chi_0\rangle$ and $|\chi_1\rangle$ with energy 0 and σ. Then its Hamiltonian can be represented as $H_q=\sigma A^\dagger A$, where A is the lowering operator satisfying $A|\chi_0\rangle=0$ and $A|\chi_1\rangle=|\chi_0\rangle$. In addition, the interaction term $H_{\text{int.}}$ can be taken to be

$$H_{\text{int.}}=\epsilon(t)\int\mathrm{d}^3x\,\hat{\phi}(\mathbf{x})\big(F(\mathbf{x})A+\text{h.c.}\big), \tag{41}$$

with $F\in C_0^\infty(\mathbb{R}^3)$. The coupling $\epsilon\in C_0^\infty(R)$ is opened and closed slowly and is nonzero during a finite range of time.

Now we would like to calculate the quantum transition of the system using the time-dependent perturbation theory to the leading order in ϵ. We choose the interaction picture such that field operators have the same time revolution as free fields. In particular, we have $A_{\text{I}}(t)=e^{-\mathrm{i}\sigma t}A_{\text{S}}$, and

$$(H_{\text{int.}})_{\text{I}}=\epsilon(t)\int\mathrm{d}^3x\,\big(e^{-\mathrm{i}\sigma t}F(\mathbf{x})\hat{\phi}_{\text{I}}(t,\mathbf{x})A_{\text{S}}+\text{h.c.}\big). \tag{42}$$

We assume that the system is initially in the state

$$|\Psi_\mathrm{i}\rangle = |\chi\rangle|n_\psi\rangle, \qquad \text{with} \quad |n_\psi\rangle \equiv (0,\cdots,0,\psi^{a_1}\cdots\psi^{a_n},0,\cdots) \tag{43}$$

where a_i's are Fock indices. Then at the end of the evolution, namely, a long time after turning off the coupling, the initial state $|\Psi_\mathrm{i}$ becomes

$$|\Psi_\mathrm{f}\rangle = \bigg(I - \mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t (H_\mathrm{int})_\mathrm{I}\bigg)|\Psi_\mathrm{i}\rangle. \tag{44}$$

Note that

$$\int_{-\infty}^{+\infty} \mathrm{d}t\, (H_\mathrm{int.})_\mathrm{I} = \hat{\psi}_I(f) A_\mathrm{S}, \tag{45}$$

with $f(t,\mathbf{x}) = \epsilon(t)e^{-\mathrm{i}\sigma t}F(\mathbf{x})$ is a complex test function[2]. Here we can replace the operator in interaction picture with ones in Heisenberg picture, up to a ϵ^2 term. Thus,

$$\psi_\mathrm{I}(f) \simeq \psi_\mathrm{H}(f) = \mathrm{i}a(\overline{KE\bar{f}}) - \mathrm{i}a^\dagger(KEf). \tag{46}$$

Since the coupling is turned on and turned off adiabatically, the coupling should changes with time so slow that f is function of almost positive frequency. Then we have $KEf \simeq Ef \equiv -\lambda$ and $KE\bar{f} \simeq 0$, and $\phi_\mathrm{I}(f) \simeq \mathrm{i}a^\dagger(\lambda)$. Substitute this back into (44), we find

$$|\Psi_f\rangle = \big(I + a^\dagger(\lambda)A - a(\bar{\lambda})A^\dagger\big)|\Psi_i\rangle = |\chi\rangle|n_\psi\rangle + \sqrt{n+1}\|\lambda\|(A|\chi\rangle)|(n+1)'\rangle \tag{47}$$

3 Quantum Fields in Curved Spacetime

In this section we mainly consider the Klein-Gordon field ϕ defined over a spacetime $(\mathscr{M}, g_{ab})$. In our treatment the spacetime metric g_{ab} is regarded as a background field and its dynamics is irrelevant to us, except when we study the back reaction of the Klein-Gordon field on the metric.

3.1 Constructing quantum fields in curve spacetimes

The classical action of the Klein-Gordon field is given by

$$S = -\frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}\big(\nabla_a\phi\nabla^a\phi + m^2\phi^2 - \xi R\phi^2\big), \tag{48}$$

where ∇_a is the covariant derivative adapted to the metric g_{ab}, R is the scalar curvature and ξ is the coupling constant which can also be set to zero if one does not wish to consider this term. In the following we will always take $\xi = 0$ although the results also hold for nonzero ξ.

To construct a physically meaningful quantum field theory, we must put additional constraint on the background spacetime $(\mathscr{M}, g_{ab})$. In particular, we except the spacetime to have a good causal structure such that an initial value problem can be formulated. For this purpose, the spacetime will be taken to be globally hyperbolic. This requirement is equivalent to the existence of a Cauchy surface Σ whose domain of dependence is the whole spacetime. In addition, if $(\mathscr{M}, g_{ab})$ is globally hyperbolic with Cauchy surface Σ, then $\mathscr{M}$ is topologically equivalent to $\mathbb{R}\times\Sigma$, and can be foliated by a one-parameter family of smooth Cauchy surface Σ_t. That is, a smooth time

[2]Therefore $\phi_\mathrm{I}(f)$ should be understood as $\phi_\mathrm{I}(\mathrm{Re}\, f) + \mathrm{i}\phi_\mathrm{I}(\mathrm{Im}\, f)$.

coordinate t can be chosen on $\mathscr{M}$ such that each surface of constant t is a Cauchy surface. See Chapter 8 in [3] for more details.

In such a globally hyperbolic spacetime, we can formulate a well-defined classical system of field. This can be stated more precisely by the following theorem (see [4] for more details):

Theorem. *Let $(\mathscr{M}, g_{ab})$ be a globally hyperbolic spacetime with smooth, spacelike Cauchy surface Σ. Then the Klein-Gordon equation:*

$$\nabla^a\nabla_a\phi - m^2\phi = 0 \tag{49}$$

has a well posed initial value formulation in the following sense: Given any pair of C^∞ functions $(\phi_0, \dot{\phi}_0)$ on Σ, there exits a unique solution ϕ to the Klein-Gordon equation, such that on Σ we have $\phi = \phi_0$ and $n^a\nabla_a\phi = \dot{\phi}_0$, where n^a denotes the future directed unit vector normal to Σ. Furthermore, for any closed subset $S \subset \Sigma$, the solution ϕ restricted to $D(S)$ depends only upon the initial data on S. In addition, ϕ is smooth and varies continuously with the initial data.

A source term f can be added to the Klein-Gordon equation without affecting the above theorem. Thus the theorem implies that there exist unique advanced and retarded solutions to the Klein-Gordon equation with given source.

With a globally hyperbolic spacetime $(\mathscr{M}, g_{ab})$, now we are going to formulate the classical and quantum theory of Klein-Gordon field. We first introduce the global time function t and use it to slice $\mathscr{M}$ into Cauchy surfaces Σ_t. Then we define the time evolution vector field t^a on $\mathscr{M}$ by $t^a\nabla_a t = 1$ and decompose it as

$$t^a = Nn^a + N^a, \tag{50}$$

with n^a the unit normal to Σ_t, called *lapse function*, and N^a tangent vector of Σ_t, called *shift vector*. Then the local coordinate (t, x^1, x^2, x^3) can be introduced such that $t^a = (\partial/\partial t)^a$ and $t^a\nabla_a x^i = 0$ $(i = 1, 2, 3)$. In this coordinate the action for Klein-Gordon field (48) can be written as $S = \int \mathrm{d}t\, L$, with the Lagrangian given by

$$L = \frac{1}{2}\int_{\Sigma_t} \mathrm{d}^3x\,\sqrt{h}N\big((n^a\nabla_a\phi)^2 - h^{ab}(\nabla_a\phi)(\nabla_b\phi) - m^2\phi^2\big), \tag{51}$$

with h_{ab} the metric induced from g_{ab} on Σ_t.

Now, from $n^a\nabla_a\phi = N^{-1}(t^a - N^a)\nabla_a\phi = N^{-1}(\dot{\phi} - N^a\nabla_a\phi)$, we find the momentum density $\dot{\phi}$ conjugate to ϕ on Σ_t is given by $\pi = (n^a\nabla_a\phi)\sqrt{h}$. Then, the classical phase space is again spanned by all test function pairs (ϕ, π) on Σ_0, namely (34), and the symplectic product is given by (35). With the explicit form of π, we can further rewrite (35) as

$$\Omega\big((\phi_1, \pi_1), (\phi_2, \pi_2)\big) = \int_{\Sigma_0} \mathrm{d}^3x\,\sqrt{h}\big(\phi_2 n^a\nabla_a\phi_1 - \phi_1 n^a\nabla_a\phi_2\big). \tag{52}$$

The identification between the solution space $\mathscr{S}$ and the phase space $\mathscr{M}$ still holds now, and we can use the former as the starting point of quantization. All steps are the same with that in Subsection 2.4, except that now there is no definite meaning of positive or negative frequency solutions. Naïvely, we are free to choose any subspace $\mathscr{S}^{\mathbb{C}+} \subset \mathscr{S}^{\mathbb{C}}$ satisfying three conditions imposed in Subsection 2.3 to complexify it into a Hilbert space $\mathscr{H}$, and take this $\mathscr{H}$ as the one-particle space and define the quantum state space to be $F_S(\mathscr{H})$. Actually the fact is that the choice is a little more complicated for field theories due to infinitely many degrees of freedom, which will be explained in the next section. But, anyway, the ambiguity remains.

The ambiguity of choosing the one-particle space $\mathscr{H}$ has two important consequences. One is that the concept of particles loses its meaning in general cases. That is, a one-particle state associated with a given choice of $\mathscr{H}$ may not be a one-particle state in another choice of $\mathscr{H}$. In particular, the vacuum associated with a given $\mathscr{H}$ may fail to be a vacuum state with other choices. However, as will be seen in the next subsection, in a stationary spacetime, or in asymptotic regions of a asymptotically stationary spacetime, the concept of particle still works well.

The other consequence is that different choices of one-particle space for a field system with infinitely many degrees of freedom will in general lead to unitarily inequivalent representations of Weyl relations. The resulted quantum theories will give distinct physical predictions, except when there are criteria telling us how to pick out a preferred choice of one-particle space. Criteria of this kind exist in some cases, e.g., when the spacetime is stationary, the time function gives an unambiguous set of positive frequency solutions to classical equation of motion, with which the one-particle space is spanned; when the Cauchy surface of the spacetime is compact, the so-called Hadamard condition on quantum states also picks out a preferred choice for one-particle space. But in general, there is no such criteria. Therefore it is of great interest and importance to know how should one describe this ambiguity. In the next subsection, we will introduce additional mathematical settings with which one can describe the ambiguity from different but equivalent perspectives.

3.2 Ambiguous one-particle spaces

Now we are going to study the problem that what freedom is available for us in the choice of the one-particle space $\mathscr{H}$. To begin with, let's recall the three condition we gave when studying the harmonic oscillators in Subsection 2.3. In that case, the one-particle space $\mathscr{H}$ is picked out from the complexified solution space $\mathscr{S}^{\mathbb{C}}$, equipped with a bilinear form (20), satisfying the three conditions:

1. The bilinear map $(,)$ defined via (20) is positively definite on $\mathscr{H}$;
2. $\mathscr{S}^{\mathbb{C}}$ is spanned by $\mathscr{H}$ and $\bar{\mathscr{H}}$;
3. $\forall y^+ \in \mathscr{H}$ and $\forall y^- \in \bar{\mathscr{H}}$, we have $(y^+, y^-) = 0$.

But these conditions are no longer that useful in field theories since now $\mathscr{S}^{\mathbb{C}}$ is a space of infinite dimensions. More explicitly, if we are going to identify the Hilbert space $\mathscr{H}$ as a subspace of $\mathscr{S}^{\mathbb{C}}$, we should Cauchy-complete the latter in advance. But the process of Cauchy-completeness requires an inner product which can be borrowed from $\mathscr{H}$ only. But this is already a partial specification of $\mathscr{H}$. For this reason we will introduce another way of characterizing the choice of $\mathscr{H}$ now.

No matter which way we take, we must face with the task of Cauchy-completing, which needs a structure of inner product. Thus we could begin with defining an inner product directly on $\mathscr{S}$. To motivate how should we define it, let's go back to the case of harmonic oscillators. Suppose now we have found the one-particle space $\mathscr{H} \subset \mathscr{S}^{\mathbb{C}}$ consisting of positive frequency modes, as was done in Subsection 2.3. Then, we define a bilinear form $\mu : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$, as

$$\mu(y_1, y_2) \equiv \mathrm{Re}\,(Ky_1, Ky_2)_{\mathscr{H}} = \mathrm{Im}\,\Omega(\overline{Ky_1}, Ky_2), \qquad \forall y_1, y_2 \in \mathscr{S}, \tag{53}$$

where $K : \mathscr{S} \to \mathscr{H}$ is the projection operator projecting a solution to its positive frequency component. The bilinear form μ defined in this way is positively definite. To see this, we note that

$$\mathrm{Im}(Ky_1, Ky_2) = -\mathrm{Re}\,\Omega(\overline{Ky_1}, Ky_2) = -\tfrac{1}{2}\big(\Omega(\overline{Ky_1}, Ky_2) + \Omega(Ky_1, \overline{Ky_2})\big) = -\tfrac{1}{2}\Omega(y_1, y_2). \quad (54)$$

Then,

$$(Ky_1, Ky_2)_{\mathscr{H}} = \mathrm{Re}\,(Ky_1, Ky_2)_{\mathscr{H}} + \mathrm{i}\,\mathrm{Im}\,(Ky_1, Ky_2)_{\mathscr{H}} = \mu(y_1, y_2) - \tfrac{1}{2}\Omega(y_1, y_2). \quad (55)$$

Now we apply the Schwartz inequality,

$$\|z_1\|^2\|z_2\|^2 \geq |(z_1, z_2)|^2 \geq |\,\mathrm{Im}\,(z_1, z_2)|^2, \qquad \forall z_1, z_2 \in \mathscr{H},$$

with $z_1 = Ky_1$ and $z_2 = Ky_2$, to get

$$\mu(y_1, y_1)\mu(y_2, y_2) \geq \tfrac{1}{4}\Omega^2(y_1, y_2). \quad (56)$$

Therefore μ is positive definite and is really a inner product. Actually, since the equality in the expression above can always be reached, we can write down a stronger condition on μ, namely:

$$\mu(y_1, y_2) = \frac{1}{4}\max_{y_2 \neq 0}\frac{\Omega^2(y_1, y_2)}{\mu(y_1, y_2)}. \quad (57)$$

This condition is strong enough, in the sense that any inner product on $\mathscr{H}$ satisfying it will give rise to a one particle space $\mathscr{H}$. To see this, suppose μ is an inner product on $\mathscr{H}$ satisfying (57). Then we claim that for each $y_1 \in \mathscr{S}$, there exists a unique $y_2 \in \mathscr{S}$, such that the following two equalities hold:

$$\tfrac{1}{2}\Omega(y_1, y_2) = \mu(y_1, y_1), \qquad \text{and} \qquad \mu(y_2, y_2) = \mu(y_1, y_1). \quad (58)$$

Otherwise, suppose both y_2 and y_2' with $y_2 \neq y_2$ satisfy the equalities above, then we evaluate the following expression with $y_2'' = y_2 + y_2'$:

$$\frac{\Omega^2(y_1, y_2'')}{4\mu(y_2'', y_2'')} = \frac{\mu^2(y_1, y_1)}{2\mu(y_1, y_1) + 2\mu(y_2, y_2')} > \frac{\mu^2(y_1, y_1)}{2\mu(y_1, y_1) + 2\mu(y_1, y_1)} = \mu(y_1, y_2),$$

where we have applied the Schwartz inequality again. But this expression contradicts (57). Then the uniqueness of y_2 follows. Now, $\forall y_1 \in \mathscr{S}$, let $y_2 \in \mathscr{S}$ be the unique element associated with y_1 in the way described above. Then, we claim that the one-particle space $\mathscr{H}$ is given by $\mathscr{H} = \{\tfrac{1}{2}(y_1 + \mathrm{i}y_2) | y_1 \in \mathscr{S}\}$. It can be checked that $\mathscr{H}$ defined in this way satisfies all three conditions list at the beginning of this subsection. (Check it!)

Now let's turn to field theories. As argued above, the three conditions on $\mathscr{H}$ is not suitable in this case. However, the inner product on $\mathscr{S}$ defined above can be generalized directly to field theories. To achieve this, we only need to replace (57) with the following condition:

$$\mu(\psi_1, \psi_1) = \frac{1}{4}\underset{\psi_2 \neq 0}{\mathrm{l.u.b.}}\frac{\Omega^2(\psi_1, \psi_2)}{\mu(\psi_2, \psi_2)}, \quad (59)$$

where "max" has been replaced with "l.u.b.", namely the least upper bound, since the maximum may not be reached due to the continuously many dimensions. We will show that such an inner product will generate a desired one-particle space $\mathscr{H}$.

We begin with Cauchy-completing the solution space $\mathscr{S}$ with respect to the inner product $(\cdot,\cdot)$ defined as $(\psi_1,\psi_2)=2\mu(\psi_1,\psi_2)$, with the coefficient 2 merely a normalization factor. Then, the completed space $\mathscr{S}_\mu$ is a real Hilbert space. From (59) we see that the symplectic form Ω is bounded on $\mathscr{S}$ with respect to its inner product. Thus we can generalize Ω to $\mathscr{S}_\mu$ in a continuous way.

Now we define the operator $\mathscr{S}_\mu\to\mathscr{S}_\mu$, according to

$$\Omega(\psi_1,\psi_2)=2\mu(\psi,J\psi_2)=(\psi_1,J\psi_2). \tag{60}$$

The anti-symmetry of Ω immediately implies that $J^\dagger=-J$. On the other hand, (59) is equivalent to the statement that $J^\dagger J=I$. (Why??) Therefore we have $J^2=-I$ and thus J gives rise to a complex structure on $\mathscr{S}$. Conversely, given a complex structure J on $\mathscr{S}$ such that $-\Omega(\psi_1,J\psi_2)$ is a positive definite bilinear map, we have naturally an inner product μ defined via (60). Therefore we have a rough correspondence between the inner product μ defined on $\mathscr{S}$ satisfying (59), and the complex structure J defined on $\mathscr{S}$. It is a rough because the complex structure generated by μ is in general defined on $\mathscr{S}_\mu$ rather on $\mathscr{S}$.

Now, let's complexify $\mathscr{S}_\mu$ together with its structures Ω, μ, and J. We define the inner product on $\mathscr{S}_\mu^{\mathbb{C}}$ to be

$$(\psi_1,\psi_2)\equiv 2\mu(\bar{\psi}_1,\psi_2),\qquad \forall\psi_1,\psi_2\in\mathscr{S}_\mu^{\mathbb{C}}, \tag{61}$$

which makes $\mathscr{S}_\mu^{\mathbb{C}}$ a complex Hilbert space. Note that $\mathrm{i}J:\mathscr{S}_\mu^{\mathbb{C}}\to\mathscr{S}_\mu^{\mathbb{C}}$ is self-adjoint, thus from the spectrum theorem we know that $\mathscr{S}_\mu^{\mathbb{C}}$ can be decomposed into two eigenspaces of J with eigenvalues $\pm\mathrm{i}$. Now, we define the one-particle space $\mathscr{H}$ to be the eigenspace of J with eigenvalue $+\mathrm{i}$, then it can be shown (Show it!) that this $\mathscr{H}$ satisfies the three defining conditions, except that we should replace $\mathscr{S}^{\mathbb{C}}$ with $\mathscr{S}_\mu^{\mathbb{C}}$ in Condition 2. In addition, we can define the orthogonal projection $K:\mathscr{S}_\mu^{\mathbb{C}}\to\mathscr{H}$. The restriction of K in $\mathscr{S}$ is a real linear map $K:\mathscr{S}\to\mathscr{H}$, with $K(\mathscr{S})$ a dense subset of $\mathscr{H}$. Furthermore, we have

$$(K\psi_1,K\psi_2)_{\mathscr{H}}=-\mathrm{i}\Omega(\overline{K\psi_1},K\psi_2)=\mu(\psi_1,\psi_2)-\tfrac{1}{2}\mathrm{i}\Omega(\psi_1,\psi_2). \tag{62}$$

In particular,

$$\operatorname{Im}(K\psi_1,K\psi_2)_{\mathscr{H}}=\tfrac{1}{2}\Omega(\psi_1,\psi_2). \tag{63}$$

Conversely, given a one-particle space $\mathscr{H}$ and a real linear map $K:\mathscr{S}\to\mathscr{H}$ satisfying the equation above and the condition that $K(\mathscr{S})$ is dense in $\mathscr{H}$, one can find an inner product μ on $\mathscr{S}$ satisfying (59). Thus we have established the correspondence between choosing the one-particle space and choosing the inner product on $\mathscr{S}$.

3.3 Quantum field theory in stationary spacetimes

Now let's consider the stationary spacetime. By stationary we mean a spacetime which admits a one-parameter group of isometries with timelike orbits. Let ξ^a be the Killing vector field generating the isometries and define the Killing time t to be a global function over the spacetime satisfying $\xi^a\nabla_a t=1$. Then we may attempt to Fourier decompose the solution of classical equations of motion into positive and negative frequency parts with respect to Killing time. But the Fourier resolution needs the structure of hypersurface-orthogonality of the Killing field, which is the case in a static spacetime but not in a stationary spacetime. (The static spacetime by definition is a stationary spacetime with hypersurface-orthogonal Killing field. See [3] and [5] for details.) Therefore we will take another way to the positive frequency one-particle space $\mathscr{H}$ without using Fourier resolution, following [5].

For technique reasons, we introduce two additional conditions. One is on the field: we need the Klein-Gordon field to be massless, namely $m > 0$, to avoid troubles from infrared divergence. The other is on the spacetime: we assume that there exists a Cauchy surface Σ such that on Σ we have

$$-\xi^a\xi_a \geq -\epsilon\xi^a n_a > \epsilon^2, \tag{64}$$

for some $\epsilon > 0$.

The original idea of [5] on seeking for the one-particle space is from the observation that a positive frequency solution $\psi^+ \in \mathscr{H}$ is not only a solution of classical field equation, but also a one-particle state in the quantum Fock space. Therefore there are two ways two evaluate the stress-energy tensor associated with ψ^+: One is to substitute the solution into the classical expression for the stress tensor T_{ab}, and the other is to calculate the expectation value $\langle\psi|T_{ab}|\psi\rangle$. It is suggested in [5] that both evaluations should give the same answer, thus fixes the choice of $\mathscr{H}$. It is further proved that the one-particle space $\mathscr{H}$ found in this way does coincide with the space of positive-frequency solutions.

In light of this consideration, we define a bilinear map $\langle\cdot,\cdot\rangle$ on $\mathscr{S}^{\mathbb{C}}$, called energy inner product, by

$$\langle\psi_1,\psi_2\rangle = \int_\Sigma \mathrm{d}^3x\,\sqrt{h}T_{ab}\xi^a n^b, \tag{65}$$

with the stress tensor T_{ab} defined via

$$T_{ab}(\psi_1,\psi_2) = \nabla_{(a}\bar{\psi}_1\nabla_{b)}\psi_2 - \frac{1}{2}g_{ab}\big(\nabla^c\bar{\psi}_1\nabla_c\psi_2 + m^2\bar{\psi}_1\psi_2\big). \tag{66}$$

The bilinear function defined above is independent of Killing time t. To see this, we note that the stress tensor satisfies $T_{ab} = T_{ba}$ and $\nabla^a T_{ab} = 0$, as can be checked directly from the expression above with ψ_1 and ψ_2 are solutions of classical field equation. We also note that the Killing field ξ^a satisfies the Killing equation $\nabla_{(a}\xi_{b)} = 0$. Combining all these facts we see that $\nabla^a(T_{ab}\xi^b) = 0$. Then, we perform the following integration with the integral region the spacetime within two Cauchy surfaces Σ_1 and Σ_2 located at $t = t_1$ and $t = t_2$, respectively:

$$0 = \int_{\Sigma_1}^{\Sigma_2} \mathrm{d}t\mathrm{d}^3x\sqrt{g}\nabla^a(T_{ab}\xi^b) = \int_{\Sigma_2}\mathrm{d}^3x\,\sqrt{h}T_{ab}n^a\xi^b - \int_{\Sigma_1}\mathrm{d}^3x\,\sqrt{h}T_{ab}n^a\xi^b.$$

This shows that the energy inner product $\langle\cdot,\cdot\rangle$ is indeed time independent. Furthermore, it can be checked that $\langle\cdot,\cdot\rangle$ is indeed a inner product in that it is positively definite.

Then we can Cauchy-complete $\mathscr{S}^{\mathbb{C}}$ in the norm defined by $\langle\cdot,\cdot\rangle$ to get a Hilbert space $\tilde{\mathscr{H}}$, and the time translation on $\tilde{H}$ is a one-parameter group of strongly continuous unitary transformations $V + t$. From Stone theorem V_t has the form $e^{-\mathrm{i}\tilde{h}t}$ with $\tilde{h} : \tilde{H} \to \tilde{H}$ a self-adjoint operator, which generates time translation, namely,

$$\tilde{h}\psi = \mathfrak{L}_\xi\psi, \tag{67}$$

where $\mathfrak{L}_\xi$ is the Lie derivative associated with ξ^a.

Now we define a bilinear map $B : \mathscr{S}^{\mathbb{C}} \to \mathscr{S}^{C}$ by $B(\psi_1, \psi_2) = \Omega(\bar{\psi_1}, \psi_2)$. Then, from the definition of Ω, (35), and the two assumptions made above, one can prove (Prove it!) that

$$|B(\psi_1, \psi_2)| \leq C\|\psi_1\|\|\psi_2\|. \tag{68}$$

Thus B is bounded, and can be generalized to $\tilde{H}$ continuously. In addition, we can check directly from definition that

$$B(\psi_1, \tilde{\psi_2}) = 2\mathrm{i}\langle\psi_1, \psi_2\rangle. \tag{69}$$

This two equations, together with the fact that $\mathscr{S}^C$ is dense in $\mathscr{H}$, implies that the spectrum of $\tilde{h}$ is bounded away from zero, and thus $\tilde{h}^{-1}$ exists and is also bounded on $\mathscr{H}$.

Now we take $\tilde{\mathscr{H}}^+$ to be the subspace of $\tilde{H}$ with positive spectrum of $\tilde{h}$, then by (67), $\tilde{\mathscr{H}}^+$ can be interpreted as the space of positive frequency modes. Let $K : \tilde{\mathscr{H}} \to \tilde{\mathscr{H}}^+$ to be the orthogonal projection, and for $\forall\psi_1, \psi_2 \in \mathscr{S}$, define $\mu : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$ via

$$\mu(\psi_1, \psi_2) = \mathrm{Im}\, B(K\psi_1, K\psi_2) = 2\mathrm{Re}\,\langle K\psi_1, \tilde{h}^{-1}K\psi_2\rangle, \tag{70}$$

then it can be shown (Show it!) that μ satisfies (59), and thus $\tilde{H}^+$ is the desired one-particle space.

One can show that the particle interpretation made in Subsection 2.5 still works here. Therefore the concept of particles can be well defined in a globally hyperbolic stationary spacetime.

Now we consider spacetimes of partially stationary or asymptotically stationary. Let's consider first a spacetime $(\mathscr{M}, g_{ab})$ which is stationary in the past. More precisely, there exist a Cauchy surface Σ, and another globally hyperbolic stationary spacetime $(\mathscr{M}', g'_{ab})$ with a Cauchy surface $\Sigma' \subset \mathscr{M}$, such that $I^-(\Sigma)$ is isometric $I^-(\Sigma')$. In this case, one can identify the two solution spaces $\mathscr{S}$ and $\mathscr{S}'$, by identifying a solution $\psi \in \mathscr{S}$ with $\psi' \in \mathscr{S}'$ if $\psi\big|_{I^-(\Sigma)} = \psi'\big|_{I^-(\Sigma')}$. Then, we can borrow the one-particle space $\mathscr{H}'$ from $\mathscr{S}'$ and treat it as the one-particle space in the past of Σ on $\mathscr{M}$. We will denote this one-particle space by $\mathscr{H}_{\mathrm{in}}$. Similarly, if solutions on a spacetime $\mathscr{M}$ are asymptotically equal to ones on another globally hyperbolic stationary spacetime $\mathscr{M}'$ as the time goes to negative infinity, we can also identify the two solution space properly, and use this identification to build a one-particle space $\mathscr{H}_{\mathrm{in}}$.

In the same way, we can also construct $\mathscr{H}_{\mathrm{out}}$. Now if the spacetime $\mathscr{M}$ is or approaches to stationary spacetime in both of time directions, then we can construct $\mathscr{H}_{\mathrm{in}}$ and $\mathscr{H}_{\mathrm{out}}$ simultaneously. Furthermore, if $\mathscr{H}_{\mathrm{in}}$ and $\mathscr{H}_{\mathrm{out}}$ are unitarily equivalent, then there exists a unitary transformation $U : F_S(\mathscr{H}_{\mathrm{in}}) \to F_S(\mathscr{H}_{\mathrm{out}})$. This unitary map is conventionally called the S-matrix.

With the formalism built in this subsection, we can prove that for each Klein-Gordon field in a globally hyperbolic spacetime, one can always find an inner product $\mu : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$ defined on the solution space $\mathscr{S}$. Thus the quantum field theory constructed as described in Subsection 3.2 always exists. (To be complete)

3.4 The S-matrix

Let $(\mathscr{S}, \Omega)$ be an arbitrary symplectic space. In particular, we would expect $\mathscr{S}$ to be the space of solutions of classical Klein-Gordon equation. Let $\mu_1 : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$ and $\mu_2 : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$ be two inner products satisfying the condition (59). We know from previews subsections that μ_1 and μ_2 determine two one-particle spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, and thus two quantum state space $\mathscr{F}_1 = F_S(\mathscr{H}_1)$ and $\mathscr{F}_2 = F_S(\mathscr{H}_2)$ together with quantum operators of canonical variables $\widehat{\Omega}_1(\psi, \cdot) : \mathscr{F}_1 \to \mathscr{F}_1$

and $\widehat{\Omega}_2(\psi,\cdot):\mathscr{F}_2\to\mathscr{F}_2$. The problem we address here is that under what conditions the two constructions of quantum field theory are unitarily equivalent, i.e., there exists a unitary map $U:\mathscr{F}_1\to\mathscr{F}_2$, such that $\forall\psi\in\mathscr{S}$, we have

$$U\widehat{\Omega}_1(\psi,\cdot)U^{-1}=\widehat{\Omega}_2(\psi,\cdot). \tag{71}$$

This problem is important both theoretically and practically, for, it not only tells us how to choose the inner products on $\mathscr{S}$ to construct equivalent or inequivalent theories, but also gives the S-matrix for a asymptotically stationary spacetime.

We distinguish two cases: 1) There exits $C,C'>0$ such that $\forall\psi\in\mathscr{S}$, we have

$$C\mu_1(\psi,\psi)\le\mu_2(\psi,\psi)\le C'\mu_1(\psi,\psi). \tag{72}$$

2) No such C and C' exist. We now show that two inner products of case 2 cannot lead to equivalent quantum field theories. In fact, if there does not exist a $C>0$ such that $\forall\psi\in\mathscr{S}$ we have $\mu_1(\psi,\psi)\le\mu_2(\psi,\psi)/C$, then we can find a series $\{\psi_n\}$ such that $\mu_1(\psi_n,\psi_n)=1$ for all n while $\mu_2(\psi_n,\psi_n)\to 0$ as $n\to\infty$. Then, from our analysis before, for all fixed $\psi\in\mathscr{S}$, $|\Omega(\psi,\psi_n)|^2\le\mu_2(\psi_n,\psi_n)\mu_2(\psi,\psi)\to 0$ as $n\to\infty$. Then, the quantum operator $e^{\mathrm{i}\widehat{\Omega}_2(\psi_n,\cdot)}-I$ converges strongly to zero, i.e., when applying this operator to any fixed state in $\mathscr{F}_2$, the resulted series of states tends toward zero. However, the series of states $(e^{\mathrm{i}\widehat{\Omega}_1(\psi,\cdot)}-I)|0\rangle_1$ does not tends to zero. Now, if there exists a unitary map $U:\mathscr{F}_1\to\mathscr{F}_2$, then $U|0\rangle_1\in\mathscr{F}_2$ would contradict the strong convergence of $e^{\mathrm{i}\widehat{\Omega}_2(\psi_n,\cdot)}-I$.

Therefore we only need to consider Case 1). This condition, namely (71), says nothing but that μ_1 and μ_2 give equivalent norms. That is, a series in $\mathscr{S}$ is a Cauchy series with μ_1, if and only if it is also a Cauchy series with μ_2. As a consequence, μ_1 and μ_2 lead to the same Cauchy-completed space of $\mathscr{S}$, which we will denote as $\mathscr{S}_\mu$ with no distinction between 1 and 2. Thus the two one-particle spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ can be regarded as subspaces of a common space $\mathscr{S}_\mu^{\mathbb{C}}$.

Now, we define the inner product on $\mathscr{S}_\mu^{\mathbb{C}}$ by $(\psi,\chi)=2\mu_1(\bar{\psi},\chi)$, then let $K:\mathscr{S}_\mu^{\mathbb{C}}\to\mathscr{H}_1$ be the orthogonal projection, and $\bar{K}:\mathscr{S}_\mu^{\mathbb{C}}\to\mathscr{H}_2$ be corresponding orthocomplement projection. Obviously we have $K+\bar{K}=I$. Similarly, we define another inner product on $\mathscr{S}_\mu^{\mathbb{C}}$ associated with μ_2, to be $2\mu_2(\bar{\psi},\chi)$, as well as corresponding projections K_2 and $\bar{K}_2$. By definition, these two constructions are unitarily equivalent, if and only if there exists a unitary transformation $U:\mathscr{F}_1\to\mathscr{F}_2$ such that $\forall\psi\in\mathscr{S}$ we have

$$U\big(\mathrm{i}a_1(\bar{K}_1\psi)-\mathrm{i}a_1^\dagger(K_1\psi)\big)U^{-1}=\mathrm{i}a_2(\bar{K}_2\psi)-\mathrm{i}a_2^\dagger(K_2\psi), \tag{73}$$

where a_1, $a_1^\dagger$ and a_2, $a_2^\dagger$ are annihilation and creation operators in $\mathscr{F}_1$ and $\mathscr{F}_2$, respectively. From complex linearity and continuity, this equation can be directly generalized to $\forall\psi\in\mathscr{S}_\mu^{\mathbb{C}}$. Now, we define the following four operators:

$$A=K_1|_{\mathscr{H}_2},\qquad B=\bar{K}_1|_{\mathscr{H}_2},\qquad C=K_2|_{\mathscr{H}_1},\qquad D=\bar{K}_2|_{\mathscr{H}_2}. \tag{74}$$

Then the unitary condition requires that $\forall\chi\in\mathscr{H}_1$, we have

$$Ua_1(\bar{\chi})U^{-1}=a_2(\bar{C}\bar{\chi})-a_2^\dagger(\bar{D}\bar{\chi})=a_2(\overline{C\chi})-a_2^\dagger(\overline{D\chi}), \tag{75}$$

where the operators with bars means complex conjugate maps, i.e., $\bar{A}:\bar{\mathscr{H}}_2\to\bar{\mathscr{H}}_1$, $\bar{B}:\bar{\mathscr{H}}_2\to\mathscr{H}_1$, $\bar{C}:\bar{\mathscr{H}}_1\to\bar{\mathscr{H}}_2$ and $\bar{D}:\bar{\mathscr{H}}_1\to\mathscr{H}_2$. From the condition (71) we see that A,B,C and D are all bounded operators. Furthermore, they satisfy more constrains that can be got directly from definition. For instance, we take $\chi, \psi \in \mathscr{H}_2$, then,

$$\begin{aligned}(\psi,\chi)_{\mathscr{H}_2} =& -\mathrm{i}\Omega(\bar{\psi},\chi) = -\mathrm{i}\Omega(\overline{K_1\psi+\bar{K}_1\psi}, K_1\chi+\bar{K}_1\chi)\\ =& (A\psi,A\chi)_{\mathscr{H}_1} - (B\psi,B\chi)_{\bar{\mathscr{H}}_1},\end{aligned} \tag{76}$$

which leads to

$$A^\dagger A - B^\dagger B = I. \tag{77}$$

Similarly, we can choose $\chi \in \mathscr{H}_2$ and $\psi \in \bar{\mathscr{H}}_2$, to get $A^\dagger\bar{B} = B^\dagger\bar{A}$ by the same calculation. Furthermore, we have $C^\dagger C - D^\dagger D = I$ and $C^\dagger\bar{D} = D^\dagger\bar{C}$.

On the other hand, we take $\psi \in \mathscr{H}_1$ and $\chi \in \mathscr{H}_2$, then

$$\begin{aligned}(\psi,A\chi)_{\mathscr{H}_1} =& -\mathrm{i}\Omega(\bar{\psi},K_1\chi) = -\mathrm{i}\Omega(\overline{K_2\psi+\bar{K}_2\psi}, K_1\chi+\bar{K}_1\chi)\\ =& -\mathrm{i}\Omega(\overline{K_2\psi},\chi) = (C\psi,\chi)_{\mathscr{H}_2}.\end{aligned} \tag{78}$$

This gives $A^\dagger = C$. In addition, we also have $\bar{B}^\dagger = -D$, by similar manipulations. We note that the relations $A^\dagger A = I + B^\dagger B$ and $C^\dagger C = I + D^\dagger D$ imply in particular that both A^{-1} and C^{-1} exist and are bounded.

In summary, the unitary transformation $U : \mathscr{F}_1 \to \mathscr{F}_2$ satisfying the following conditions:

$$1)\quad Ua_1(\bar{\chi})U^{-1} = a_2(\overline{C\chi}) - a_2^\dagger(\overline{D\chi}), \qquad \forall\chi\in\mathscr{H}_1; \tag{79a}$$

$$2)\quad A^\dagger A - B^\dagger B = I, \quad A^\dagger\bar{B} = B^\dagger A, \quad C^\dagger C - D^\dagger D = I, \quad C^\dagger\bar{D} = D^\dagger\bar{C}; \tag{79b}$$

$$3)\quad A^\dagger = C, \quad \bar{B}^\dagger = -D, \tag{79c}$$

are called the *Bogoliubov transformation.* Now we derive the condition for the existence of Bogoliubov transformation. If this transformation U exists, then its action on the vacuum state $|0\rangle_1$ in $\mathscr{F}_1$ can be expanded in $\mathscr{F}_2$ as

$$\Psi = U|0\rangle_1 = c(1,\psi^a,\psi^{ab},\psi^{abc},\cdots), \tag{80}$$

where c is a normalization coefficient, and we have assumed that the vacuum component of Ψ is nonzero, with loss of generality, as can be seen later. Now, we take $\xi \in \mathscr{H}_2$, and substitute $\chi = C^{-1}\xi$ into (79a), then we get

$$Ua_1(\overline{C^{-1}\xi}) = a_2(\bar{\sigma}) - a_2^\dagger(\mathcal{E}\bar{\xi}), \tag{81}$$

where the mapping $\mathcal{E} : \bar{\mathscr{H}}_2 \to \mathscr{H}_2$ is defined to be $\mathcal{E} \equiv \bar{D}\bar{C}^{-1}$. It's easy to see that $\mathcal{E}$ is symmetric, namely, $\bar{\mathcal{E}}^\dagger = \mathcal{E}$. Now let the operator equation above act on $\Psi = U|0\rangle_1$, then the left hand side vanishes by definition, and the right hand side can be found by noting that

$$\begin{aligned}a_2(\bar{\xi})\Psi =& c\big(\bar{\xi}_{a'}\psi^{a'}, \sqrt{2}\bar{\xi}_{a'}\psi^{a'a}, \sqrt{3}\bar{\xi}_{a'}\psi^{a'ab}, \sqrt{4}\bar{\xi}_{a'}\psi^{a'abc},\cdots\big),\\ a_2^\dagger(\mathcal{E}\xi)\Psi =& c\big(0, (\mathcal{E}\bar{\xi})^a, \sqrt{2}(\mathcal{E}\bar{\xi})^{(a}\psi^{b)}, \sqrt{3}(\mathcal{E}\bar{\xi})^{(a}\psi^{bc)},\cdots\big).\end{aligned}$$

Then we get a series of equations,

$$\bar{\xi}_{a'}\psi^{a'} = 0, \tag{82a}$$

$$\sqrt{2}\bar{\xi}_{a'}\psi^{a'a} = (\mathcal{E}\bar{\xi})^a, \tag{82b}$$

$$\sqrt{3}\bar{\xi}_{a'}\psi^{a'ab} = \sqrt{2}(\mathcal{E}\bar{\xi})^{(a}\psi^{b)}, \tag{82c}$$

$$\sqrt{4}\bar{\xi}_{a'}\psi^{a'abc} = \sqrt{3}(\mathcal{E}\bar{\xi})^{(a}\psi^{bc)}, \tag{82d}$$

etc. These equations must hold for all $\xi \in \mathscr{H}_2$. First, we immediately see that (82a) has the unique solution $\psi^a = 0$, and by induction, all components of Ψ with odd number of particles are zero. Then, if we view $\psi^{ab} : \bar{\mathscr{H}}_2 \to \mathscr{H}_2$ as a map in (82b), this equation tells us that $\psi^{ab} = \frac{1}{\sqrt{2}}\mathcal{E}$. Note that ψ^{ab}, as a component of a state, is not arbitrary: it should be symmetric and satisfy $\psi^{ab}\bar{\psi}_{ab} < \infty$. On the other hand, $\mathcal{E}$ is already symmetric. Thus (82b) has solutions if and only if $\mathcal{E}$ satisfies

$$\mathrm{tr}\,(\mathcal{E}^\dagger \mathcal{E}) < \infty. \tag{83}$$

Since C and C^{-1} are bounded, this condition is equivalent to $\mathrm{tr}\,(D^\dagger D) < \infty$, and is also equivalent to $\mathrm{tr}\,(B^\dagger B) < \infty$. This condition can also be represented with the inner products μ_1 and μ_2, which reads, the linear map $Q : \mathscr{S}_\mu \to \mathscr{S}_\mu$ defined via

$$\mu_1(\psi_1, Q\psi_2) = \mu_2(\psi_1, \psi_2) - \mu_1(\psi_1, \psi_2) \tag{84}$$

is of trace class[3].

When condition (83) is satisfied, the state $\Psi = U|0\rangle_1$ can be found by induction, to be

$$\Psi = c\Big(1, 0, \sqrt{\tfrac{1}{2}}\epsilon^{ab}, 0, \sqrt{\tfrac{3\cdot 1}{4\cdot 2}}\epsilon^{(ab}\epsilon^{cd)}, 0, \cdots\Big), \tag{85}$$

where ϵ^{ab} is the two-particle state corresponding to $\mathcal{E}$. It can be proved that this state is normalizable and the normalization constant c is determined by $\|\Psi\| = 1$, which is required by the unitary property of U. This result tells us that the spontaneous creation of particle pairs in vacuum occurs, if and only if $\epsilon^{ab} \neq 0$, namely $\mathcal{E} \neq 0$, and equivalently, $D \neq 0$. Note that $D : \mathscr{H}_1 \to \bar{\mathscr{H}}_2$. Thus the spontaneous creation of particle pairs requires that some modes of positive frequency becomes of negative frequency during the time evolution.

The action of U on other states in $\mathscr{F}_1$ can be found in similar ways. For instance, $Ua_1^\dagger(\chi)|0\rangle_\chi$ can be found by acting the conjugation of equation (79a) on $\Psi = U|0\rangle_1$. In this way and by induction, one can find the action of U on arbitrary states in $\mathscr{F}_1$. Therefore when the condition (83) holes, U can be constructed explicitly, which then establishes the following:

Theorem. Two quantum field theories constructed from inner products μ_1 and μ_2 are unitarily equivalent, if and only if the following two conditions holds: 1) $\exists C, C' > 0$ such that $\forall \psi \in \mathscr{S}$, we have $C\mu(\psi,\psi) \leq \mu_2(\psi,\psi) \leq C'(\psi,\psi)$; b) The operator Q defined in (84) is of trace class.

The condition b) can be replaced by: b$'$) $\mathrm{tr}\,(D^\dagger D) < \infty$, or by b$''$) $\mathrm{tr}\,(B^\dagger B) < \infty$.

4 The Unruh Effect

4.1 The Unruh effect in flat spacetime

In Minkowski there is a three-parameter family of inertial time translations, corresponding to the proper time translations of inertial frames boosted in three spatial directions. Since boosts do not change a positive frequency solution to negative one and vice versa, the quantum field theory constructed under any inertial time translation has the same one-particle space with other inertial ones. Therefore constructions with different inertial frames are unitarily equivalent, which is a fact we are all familiar with.

[3] An operator in Hilbert space is said to be of trace class if its trace can be defined and is finite and independent of choice of basis

However, in Minkowski spacetime there are other isometries that can serve partially as time translations, other than inertial ones. For instance, consider the one-parameter group of Lorentz boost isometries generated by the following Killing field:

$$b^a = a\left[X\left(\frac{\partial}{\partial T}\right)^a + T\left(\frac{\partial}{\partial X}\right)^a\right], \tag{86}$$

with a an arbitrary constant and T and X are globall inertial coordinates. Several orbits of this Killing field are shown in Fig. 1, from which we see that b^a fails to be globally timelike. But it is timelike within the region I given by $|X| > T$. In addition, Region I is also globally hyperbolic. Therefore we may view the Region I as an independent spacetime being globally hyperbolic and stationary, and construct quantum field theories there. By the construction described in Subsection 3.3, there is a natural concept of particles in this stationary spacetime. In particular, the vacuum state associated with this construction unambiguously is called the *Rindler vacuum*.

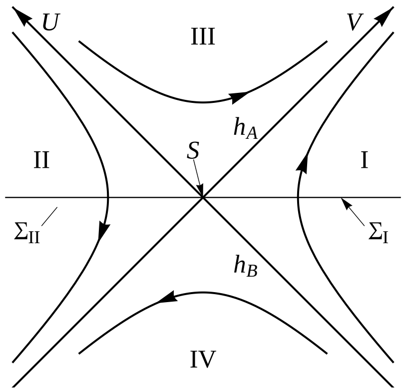

Figure 1: Unruh Effect.

From the viewpoint of an inertial observer with coordinates (T, X, Y, Z), particles at rest in frames with b^a-Killing time undergoes a motion of uniform acceleration, with different acceleration for different orbits. For the object along the orbit $b^a b_a = -1$, namely $X^2 = T^2 + a^{-2}$, it is easy to show that its 3-velocity is $w = aT\sqrt{1 + a^2T^2}$, and the spatial component of its 4-velocity if $\gamma w = aT$, with $\gamma \equiv 1/\sqrt{1 - w^2} = \sqrt{1 + a^2T^2}$. Thus its acceleration is simply a.

Now we can construct quantum field theories in two different ways. One is associated with inertial frame with global coordinates (T, X, Y, Z), the other is constructed with the time translation generated by Killing field b^a in region I. The problem we want to address is that what does the vacuum state of inertial construction, which we will called Minkowski vacuum, look like from the viewpoint of an accelerated observer? More precisely, we would like to express the Minkowski vacuum state $|0\rangle_{\mathrm{M}}$ in terms of states in Fock space associated with accelerated observers, namely, with Killing time v satisfying $b^a \nabla_a v = 1$.

For this purpose, we first construct a new quantum state space $\mathscr{F}_2 = F_S(\mathscr{H}_2)$ associated with accelerated observers, besides the inertial one which we denote as $\mathscr{F}_1 = F_S(\mathscr{H}_1)$. That is, $\mathscr{H}_2$ consists of solutions of positive frequency with respect to the Killing time v, while $\mathscr{H}_1$ consists of those with respect to the inertial time T. Now, let Σ be a Cauchy surface of the Minkowski spacetime passing through the bifurcation surface S, and let Σ_{I} and Σ_{II} be the portions of Σ in region I and region II, respectively. Then, $\mathscr{H}_2$ can be obtained by the direct sum $\mathscr{H}_2 = \mathscr{H}_{\mathrm{I}} \oplus \mathscr{H}_{\mathrm{II}}$, with $\mathscr{H}_I$ consisting of solutions with initial data with support on $\Sigma_{\rm I}$ which are positive frequency with respect to b^a, while $\mathscr{H}_2$ can be understood similarly, except that one should replace b^a with $-b^a$ since it is the latter one that is future-directed in region II. Then, we compute the action of the unitary transformation, or, the "S-matrix", $U : \mathscr{F}_1 \to \mathscr{F}_2$, on the Minkowski vacuum $|0\rangle_{\rm M}$, and formally express the result as a state in $\mathscr{F}_2$. Then we can obtain the density matrix in $\mathscr{F}_2$ corresponding to the restriction of $U|0\rangle_{\rm M}$ to region I, by tracing over the states in $F_S(\mathscr{H}_{\rm II})$. (Note that $\mathscr{F}_2 = F_S(\mathscr{H}_2) \cong F_S(\mathscr{H}_{\rm I}) \otimes F_S(\mathscr{H}_{\rm II})$.)

Now we calculate the desired density matrix following the way outlined above. First, we introduce two null coordinates for inertial observers, as

$$U = T - X, \qquad\qquad V = T + X. \tag{87}$$

A solution to the Klein-Gordon equation is in $\mathscr{H}_1$, namely, it is of positive frequency with respect to T, if and only if it is also of positive frequency with respect to U, (or equivalently, to V). Furthermore, there is a simple relation between the inertial null time V and the Killing time v on the null surface h_A, where v is determined by $b^a\nabla_a v = 1$ when $x > 0$ and by $-b^a\nabla_a v = 1$ when $x < 0$. To see this, we first rewrite b^a in (86) in terms of inertial null coordinates, as

$$b^a = a\Big[-U\Big(\frac{\partial}{\partial U}\Big)^a + V\Big(\frac{\partial}{\partial V}\Big)^a\Big]. \tag{88}$$

On h_A we have $U = 0$, then $b^a\nabla_a v = 1$ becomes $aV\partial v/\partial V = 1$ when $x > 0$, which can be easily solved. When combined with result with $x < 0$, it can be written as

$$v = \frac{1}{a}\log|V|. \tag{89}$$

Similarly, on h_B we have $u = -a^{-1}\log|U|$, where u is again the Killing time on h_B.

The general strategy to find the unitary transformation $U : \mathscr{F}_1 \to \mathscr{F}_2$, or equivalently, to find relevant Bogoliubov coefficients, is to expand the plane waves in Minkowski spacetime in terms of positive frequency modes with respect to Rindler time, and to do the reverse expansion also. But at this stage, following Wald [1], we will use a trick to free us from doing all these somewhat complicated expansions. A crucial ingredient for this trick is that any solution to the Klein-Gordon equation on Minkowski spacetime is uniquely determined by its restriction to $h_A \cup h_B$. We will not present the proof of this statement here, which can be found in [6]. Then it follows that we can obtain positive and negative frequency solutions with respect to inertial time T, simply by Fourier decomposing the solutions on h_A or h_B, with respect to V or U, respectively. Similarly, we can also obtain positive or negative frequency solutions with respect to accelerating time by Fourier decomposing the solutions on h_A or h_B with respect to v or u, respectively. Therefore, we can find the S-matrix, or equivalently, the operators C and D defined in (74), by comparing the resulted positive frequency components of different time choices.

Now let $\psi_{\rm I}(\omega)$ be a solution of the Klein-Gordon equation which has a specific frequency ω with respect to Killing time v in region I, and vanishes in region II. Then, when restricted to h_A, $\psi_{\rm I}(\omega)$ becomes

$$f_{{\rm I}\omega}(V,Y,Z) = \begin{cases} g(Y,Z)e^{-{\rm i}\omega v}, & V > 0, \\ 0, & V < 0. \end{cases} \tag{90}$$

We want to resolute this function into Fourier modes with respect to inertial null time V. Let us denote the frequency variable associated with V by σ, then the Fourier modes with frequency σ is given by

$$\tilde{f}_{\mathrm{I}\omega} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}V\, f_{\mathrm{I}\omega}(V,Y,Z) e^{\mathrm{i}\sigma V} = \frac{1}{\sqrt{2\pi}} g(Y,Z) I(\sigma), \tag{91}$$

with

$$I(\sigma) = \int_0^{\infty} \mathrm{d}V\, e^{-\mathrm{i}(\omega/a)\log V} e^{\mathrm{i}\sigma V}. \tag{92}$$

In the same way, we can consider the solutions in region II. But these solutions can also be obtained from the "wedge reflection" isometry $(T,X,Y,Z) \to (-T,-X,Y,Z)$. Under this transformation, solutions $f_{\mathrm{I}\omega}$ transforms to $\bar{f}_{\mathrm{II}\omega}$, which is of mono frequency on h_A when $x<0$ and vanishes on h_A when $x>0$. That is, we have

$$\bar{f}_{\mathrm{II}\omega}(V,Y,Z) = \begin{cases} 0, & V>0, \\ g(Y,Z) e^{-\mathrm{i}\omega v}, & V<0. \end{cases} \tag{93}$$

This function can also be decomposed into modes with respect to V, as

$$\begin{aligned} \tilde{\bar{f}}_{\mathrm{II}\omega} &= \frac{1}{\sqrt{2\pi}} g(Y,Z) \int_{-\infty}^{0} \mathrm{d}V\, e^{-\mathrm{i}(\omega/a)\log|V|} e^{\mathrm{i}\sigma V} \\ &= \frac{1}{\sqrt{2\pi}} g(Y,Z) \int_0^{\infty} \mathrm{d}V\, e^{-\mathrm{i}(\omega/a)\log|V|} e^{-\mathrm{i}\sigma V} = \frac{1}{\sqrt{2\pi}} g(Y,Z) I(-\sigma). \end{aligned} \tag{94}$$

Then we see immediately that

$$\tilde{\bar{f}}_{\mathrm{II}\omega}(\sigma,Y,Z) = \tilde{f}_{I\omega}(-\sigma,Y,Z). \tag{95}$$

To relate these modes with positive or negative modes with respect to inertial null time V, we make use of the trick of symmetry analysis. Our claim is,

$$\tilde{f}_{\mathrm{I}\omega}(-\sigma,Y,Z) = -e^{-\pi\omega/a} \tilde{f}_{\mathrm{I}\omega}(\sigma,Y,Z), \qquad \sigma>0. \tag{96}$$

To prove this equation, we evaluate $I(\sigma)$ for $\sigma>0$ defined in (92), by making the substitution $V=\mathrm{i}y$ and rotating y to the positive real axis. Here we put the branch cut of logarithm to the negative real axis. Then, $\log V = \log(\mathrm{i}y) = \log y + \mathrm{i}\pi/2$, and

$$I(\sigma) = \mathrm{i}e^{\pi\omega/2a} \int_0^{\infty} \mathrm{d}y\, e^{-\mathrm{i}(\omega/a)\log y} e^{-\sigma y}. \tag{97}$$

To fine $I(-\sigma)$, we make the substitution $V=-\mathrm{i}\sigma$, and proceed in the same way, and this time we have

$$I(-\sigma) = -\mathrm{i}e^{-\pi\omega/2a} \int_0^{\infty} \mathrm{d}y\, e^{-\mathrm{i}(\omega/a)\log y} e^{-\sigma y}. \tag{98}$$

Then (96) follows straightforwardly.

Now, we define two functions F_ω F'_ω on h_A by

$$F_\omega = f_{\mathrm{I}\omega} + e^{-\pi\omega/a} \bar{f}_{\mathrm{II}\omega}, \qquad F'_\omega = f_{\mathrm{II}\omega} + e^{-\pi\omega/a} \bar{\psi}_{\mathrm{I}\omega}. \tag{99}$$

We decompose F_ω in terms of modes with respect to V. Then its negative frequency modes read:

$$\begin{aligned}\tilde{F}_\omega(-\sigma,Y,Z) &= \tilde{f}_{I\omega}(-\sigma,Y,Z)+e^{-\pi\omega/a}\tilde{\bar{f}}_{\mathrm{II}\omega}(-\sigma,Y,Z)\\ &= -\,e^{-\pi\omega/a}\tilde{f}_{\mathrm{I}\omega}(\sigma,Y,Z)+e^{-\pi\omega/a}\tilde{f}_{\mathrm{I}\omega}(\sigma,Y,Z)=0,\end{aligned} \tag{100}$$

where we have used (95) and (96). That is, F_ω is a of pure positive frequency with respect to V. In the same way, we can show that F'_ω is also of pure positive frequency. Now, definitions of the operators $C:\mathscr{H}_1\to\mathscr{H}_2$ and $D:\mathscr{H}_1\to\bar{\mathscr{H}}_2$, we have

$$CF_\omega=f_{\mathrm{I}\omega},\qquad DF_\omega=e^{-\pi\omega/a}\bar{f}_{\mathrm{II}\omega};\qquad CF'_\omega=f_{\mathrm{II}\omega},\qquad DF'_\omega=e^{-\pi\omega/a}\bar{f}_{\mathrm{I}\omega}. \tag{101}$$

Therefore,

$$DC^{-1}f_{\mathrm{I}\omega}=e^{-\pi\omega/a}\bar{f}_{\mathrm{II}\omega},\qquad\qquad DC^{-1}f_{\mathrm{II}\omega}=e^{-\pi\omega/a}\bar{f}_{\mathrm{I}\omega}. \tag{102}$$

Note that $\{f_{\mathrm{I}\omega}\}$ and $\{f_{\mathrm{II}\omega}\}$ span $\mathscr{H}_{\mathrm{I}}$ and $\mathscr{H}_{\mathrm{II}}$ respectively, which means they span $\mathscr{H}_2=\mathscr{H}_{\mathrm{I}}\oplus\mathscr{H}_{\mathrm{II}}$ together, thus we have completely determined the operator $\mathcal{E}=\bar{D}\bar{C}^{-1}$. Then according to (to be added), the corresponding two particle state is given by

$$\epsilon^{ab}=\sum_i e^{-\pi\omega_i/a}2f^{(a}_{\mathrm{I}\omega_i}f^{b)}_{\mathrm{II}\omega_i}, \tag{103}$$

which can be rewritten in Dirac notations as

$$U|0\rangle_{\mathrm{M}}=\prod_i\left(\sum_{n=0}^{\infty}e^{-n\pi\omega_i/a}|n_i\rangle_{\mathrm{I}}\otimes|n_i\rangle_{\mathrm{II}}\right) \tag{104}$$

This is the result of acting the unitary transformation U on the Minkowski vacuum state. Now we take the tensor product of it and trace over $F_S(\mathscr{H}_2)$, to get

$$\begin{aligned}\rho &= \operatorname{tr}_{F_S(\mathscr{H}_2)}\Big\{\prod_i\sum_{n=0}^{\infty}e^{-2n\pi\omega_i/a}|n_i\rangle_{\mathrm{I}}|n_i\rangle_{\mathrm{II}}\,{}_{\mathrm{II}}\langle n_i|_{\mathrm{I}}\langle n_i|\Big\}\\ &= \prod_i\sum_{n=0}^{\infty}e^{-2n\pi\omega_i/a}|n_i\rangle_{\mathrm{I}}\,{}_{\mathrm{I}}\langle n_i|\end{aligned} \tag{105}$$

This is exactly the thermal density matrix with temperature

$$T=\frac{a}{2\pi}, \tag{106}$$

which is known as the Unruh effect.

We finish this subsection with some remarks.

4.2 Killing horizons

Now we are going to generalize the previous derivation of Unruh effect to curved spacetime. Note that the derivation above depends essentially on the structure of four wedge-like regions. Thus we will at first introduce the similar structure in curved spacetime, namely the so-called "bifurcate Killing horizon".

For illustration we firstly consider the case of 2d spacetime. We recall that an isometry is defined to be a diffeomorphism of the spacetime $(\mathscr{M}, g_{ab})$ that leaves the metric g_{ab} invariant, and that a Killing vector field ξ^a is defined to be the generator of a one-parameter group of isometries. It follows directly that ξ^a satisfies $\nabla_{(a}\xi_{b)} = 0$. Another property of Killing field which is crucial here is that it is uniquely determined over the spacetime manifold by its action (of a spacetime function) on one point $p \in \mathscr{M}$ together with its induced action on the tangent space V_p to p. Stated equivalently, a Killing vector filed ξ^a on spacetime manifold $\mathscr{M}$ is uniquely specified by its value ξ^a and the value of its derivative $F_{ab} \equiv \nabla_a\xi_b = \nabla_{[a}\xi_{b]}$ at one point. This result is most easily seen from the fact that the Killing field ξ^a satisfies the following equation:

$$\nabla_c\nabla_a\xi_b = -R_{abcd}\chi^d. \tag{107}$$

Then the statement above is justified by the uniqueness of the solution to this differential equation once the initial condition is given.

Now, in 2d spacetime, suppose a Killing field ξ^a vanishes on the point p, $\xi^a(p) = 0$. then ξ^a is totally determined by the antisymmetric tensor $F_{ab} = \nabla_a\chi_b$, which has only one independent component in 2d. This single component is nothing but the coefficient of the Lie derivative of a vector, namely, $\mathfrak{L}_\xi v^a = F^a{}_b\xi^b$. The vanishing of $\xi^a(p) = 0$ simply means that p is a fixed-point of the one-parameter group of isometries, and the behavior of ξ^a within a small neighborhood of p is determined by the signature of the spacetime metric. In Riemannian case, ξ^a is the generator of rotations and its integration curves is a family of ellipses, while in Minkowskian case, xi^a generates Lorentz boosts and its integration curves are hyperbolas, which has exactly the same structure as shown in Fig. 1.

Similar things happen in $n > 2$ dimensions, if a Killing field ξ^a vanishes entirely over an $(n-2)$d spacelike surface S. In Minkowskian case, the pair of hypersurfaces h_A and h_B generated by null geodesics orthogonal to S is called a *bifurcate Killing horizon*. This bifurcate Killing horizon locally divides the spacetime into four wedges as shown in Fig. 1.

Now we introduce the concept of *surface gravity* of an arbitrary Killing horizon. A *Killing horizon* h associated with the Killing field χ^a is defined to be a null surface to which χ^a is normal. Now, by definition we have $\chi^a\chi_a = 0$ on h, thus $\nabla^b(\chi^a\chi_a)$ must be normal to h. Since χ^a itself is also normal to h, then these two vectors must be proportional, namely, there exists a function κ on h, namely the surface gravity of h, such that

$$\nabla^b(\chi^a\chi_a) = -2\kappa\chi^b. \tag{108}$$

The surface gravity can be represented in terms of the Killing field χ^a to be

$$\kappa^2 = -\tfrac{1}{2}(\nabla_a\chi_b)(\nabla^a\chi^b), \tag{109}$$

or,

$$\kappa = \lim_{p\to h} a\sqrt{-\chi^a\chi_a}, \tag{110}$$

where a is the magnitude of the proper acceleration of the orbits of χ^a in the region outside h where ξ^a is timelike, and the limit is taken to approach the horizon. The name of "surface gravity" can be understood in the asymptotically flat spacetime in which the Killing field χ^a approaches a time translation at infinity. Then one can normalize χ^a such that $\chi^a\chi_a \to -1$ at infinity. It follows directly that $\sqrt{-\chi^a\chi_a}$ is now the gravitational redshift factor, and (110) is simply the redshifted proper acceleration of orbits of χ^a near the horizon, which is equivalent in the usual sense to the concept of surface gravity.

A crucial property of the bifurcate Killing horizons is that the surface gravity κ is a constant over the whole horizon. This can be proved in two steps. Firstly, the surface gravity κ is constant along each orbit of χ^a on h, which can be directly seen by taking the Lie derivative of (108) with respect to χ^a.

It can be shown that the event horizon of a stationary black hole must be a Killing horizon, which in turn comprises a portion of a bifurcate Killing horizon, except in the "degenerating" case of vanishing surface gravity.

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