Particle Interpretations and Green Functions for a Free Scalar Field

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Abstract

The formalism of Ashtekar and Magnon for the definition of particles in quantum field theory in curved spacetime is further developed. The relation between basic objects of this formalism (e.g., the complex structure) and different Green functions is found. It allows one to derive composition laws for Green functions.

The relation of two definitions of particles is reformulated in the formalism and the base-independent Bogoljubov transformation is expressed using quantities which are derivable directly from the “in-out” Green function.
Introduction

In this paper we will investigate the notion of particles in quantum field theory in curved background and the properties of different Green functions. Quantum field theory in curved spacetime is a well known theory developed already two decades ago [3] (see also [4–7]). We will not discuss any new physical effects, but we will develop a useful mathematical framework based on [2] which, for example, allows us to derive a lot of nontrivial relations among Green functions and helps us to understand the connection of different notions of particles. Beside making a reformulation of many known facts (such as the possibility of the reconstruction of initial and final particle states from the in-out Green function [8]) in this framework, we will show a relation between the complex structure used for the definition of particles and the Hadamard Green function, and we will express a base-independent Bogoljubov transformation in terms which are derivable directly from the in-out Green function — facts which we believe are not published elsewhere.

This paper is composed of three parts. In part 1 the structure of covariant phase-space is introduced. It is based mainly on the formulation by DeWitt [9].

Part 2 defines particle representations of quantum algebra. The standard approach for the definition of particles is a decomposition of the quantum field into modes — what essentially expresses the field as a system of harmonic oscillators. This approach could be called a “brute force” approach — it depends on a choice of a base, partially in unimportant, but partially in very important, ways. There exists another, more formal, way to define particles, introduced by Ashtekar and Magnon [2]. They have used a “complex structure” on the phase space of a classical system to define particles. We will further develop this formulation, and we will show a close relation between the complex structures (and their projector operators) and different kinds of Green functions. Next we will show that a condition of diagonalization of a Hamiltonian in a particle base picks up uniquely a notion of particles. This is a slightly different condition than the one used in [2] but leads to the same particle interpretation. Finally the boundary conditions for the Feynman Green function are found (see also [8]), and different composition laws for Green functions are derived.

The last part investigates a relation between two particle interpretations which is important for scattering situations. The developed formalism allows one to define a base independent Bogoljubov transformation and using it easily find a canonical base in which Bogoljubov coefficients are diagonal [10]. Operators \( \alpha_o, \beta_o \) on the phase space which plays a role of Bogoljubov coefficients can be expressed using a single operator \( X \) as \( \alpha_o = \cosh X, \beta_o = \sinh X \) where the operator \( X \) appears in many important quantities as an in-out Green function, S-matrix or transition amplitudes. In the part 3 we also show that initial and final notions of particles are possible to reconstruct from a knowledge of a Green function which satisfies certain conditions (see also [3]). So, if we are able to construct such a Green function using other methods as, for example, a path integral, this result allows us to define a corresponding notion of particles in standard quantum theory. Finally we will find boundary conditions for the in-out Feynman Green function and other composition laws among Green functions.

1 General definitions

Covariant phase space

We will investigate a free scalar field theory. The space of histories \( \mathcal{H} \) (i.e., field configurations in spacetime) for a real scalar field is the space of real functions on a spacetime manifold \( M \). It is a vector space, and a vector index of \( \phi^x \) denotes essentially a point \( x \) in spacetime which we will usually suppress. A dot \( \cdot \) will denote a summing over these \( \infty^4 \) indexes, i.e. integration over the spacetime \( M \).

The wave operator on \( \mathcal{H} \) is

\[
F = -\bar{\cdot} g^{\alpha\delta} \Gamma_{\alpha\beta\gamma} \cdot \bar{\cdot} g^{\beta\gamma} \delta \in H^0_2.
\]  (1.1)

Here \( g^{\alpha\beta} \) is the spacetime metric, \( g^{\frac{1}{2}} = \left( \text{Det} g \right)^{\frac{1}{2}} \in S M \) is the metric volume element and \( V \) is a spacetime dependent potential.
The equation of motion is
\[ F \cdot \phi = 0 \quad . \tag{1.2} \]

We will call the space of solutions a covariant phase space \( \Gamma \). The phase space \( \Gamma \) is generally nonlinear, but for free field it forms a vector space. The vector index labels Cauchy data for the equation of motion (for example value and momentum of field on a Cauchy hypersurface). The dot “\( \circ \)” will represent contraction over these “2\( \infty \)3” indexes.

We will introduce a symplectic structure on \( \Gamma \) using the Wronskian \( \partial F[\Sigma] \) of the operator \( F \). We have for any spacetime domain \( \Omega = \langle \Sigma_f, \Sigma_i \rangle \) between two Cauchy hypersurfaces \( \Sigma_i, \Sigma_f \)
\[
\begin{align*}
\partial F[\partial \Omega] &= (\chi[\Omega] \delta) \cdot F - F \cdot (\chi[\Omega] \delta) \in H^0_2 \quad , \\
\partial F[\partial \Omega] &= \partial F[\Sigma_f] - \partial F[\Sigma_i] \quad , \\
\partial F[\Sigma] &= \tilde{\partial}F[\Sigma] - \tilde{\partial}F[\Sigma] \quad ,
\end{align*}
\tag{1.3}
\]
where \( \chi[\Omega] \) is a characteristic function of the domain \( \Omega \) and \( \tilde{\partial}F \) is defined by
\[
\begin{align*}
\tilde{\partial}F[\Sigma] &= (g^{\hat{+}} \delta[\Sigma] \bar{n}^\alpha) \tilde{d}_{\alpha} \quad , \\
\tilde{\partial}F[\Sigma] &= \tilde{\partial}F[\Sigma]^\top = \tilde{d}_\alpha (g^{\hat{+}} \delta[\Sigma] \bar{n}^\alpha) \quad .
\end{align*}
\tag{1.5}
\]
Here \( \bar{n}^\alpha \) is a future oriented normal to the hypersurface \( \Sigma \), and \( \delta[\Sigma] \) is a delta function localized on the hypersurface \( \Sigma \), i.e. for \( \psi \in \mathfrak{F} \quad M \)
\[
\int_M \psi \delta[\Sigma] q^{\hat{+}} = \int_\Sigma \psi q^{\hat{+}} \quad .
\tag{1.7}
\]
where \( q^{\hat{+}} \in \mathfrak{F} \Sigma \) is the volume element on the hypersurface \( \Sigma \).

The Wronskian defines the usual Klein-Gordon product
\[
\phi_1 \cdot \partial F[\Sigma] \cdot \phi_2 = \int_\Sigma ( (\bar{n}^\alpha d_\alpha \phi_1) \phi_2 - \phi_1 (\bar{n}^\alpha d_\alpha \phi_2) ) q^{\hat{+}} \quad .
\tag{1.8}
\]

We have for \( \phi_1, \phi_2 \in \Gamma \), using (1.3) and (1.2)
\[
\phi_1 \cdot \partial F[\Sigma_f] \cdot \phi_2 - \phi_1 \cdot \partial F[\Sigma_i] \cdot \phi_2 = \phi_1 \cdot ( (\chi[\Omega] \delta) \cdot F - F \cdot (\chi[\Omega] \delta) ) \cdot \phi_2 = 0 \quad .
\tag{1.9}
\]
So \( \partial F[\Sigma] \) is independent of \( \Sigma \) if it acts on vectors from \( \Gamma \). Therefore we can introduce a restriction \( \partial F \in \Gamma^0 \) of \( \partial F[\Sigma] \in H^0_2 \) which is not dependent on a hypersurface \( \Sigma \). \( \partial F \) is an antisymmetric nondegenerated closed bi-form on \( \Gamma \), which means it is a symplectic structure of our phase space.

We can define its inversion
\[
G_C \in \Gamma^2_0 \quad , \quad G_C^\top = -G_C \quad , \quad G_C \circ \partial F = \partial F \circ G_C = -\delta(\Gamma) \quad \tag{1.10}
\]
or, formulated on the space of histories \( H \),
\[
G_C \in H^2_0 \quad , \quad F \circ G_C = G_C \circ F = 0 \quad , \quad G_C^\top = -G_C \quad , \quad G_C \circ \partial F[\Sigma] = \partial F[\Sigma] \circ G_C = -D_C[\Sigma] \quad .
\tag{1.11}
\]
Here \( \delta(\Gamma) \) is the identity operator on \( \Gamma \) and \( D_C[\Sigma] \) propagates Cauchy data on a hypersurface \( \Sigma \) to a solution of the equation of motion (1.2). It is a projection from \( H \) to \( \Gamma \) using the Cauchy data on \( \Sigma \). It induces a mapping between spaces \( H^l_k \) and \( \Gamma^l_k \) which we will call \( \iota[\Sigma] \).
$G_C$ is called the causal Green function. It is possible to show (see [1]) that

$$G_C = G_{ret} - G_{adv} ,$$

(1.12)

where $G_{ret}, G_{adv}$ are retarded and advanced Green functions for equation (1.2).

The Poisson bracket of two observables $A, B \in \mathcal{F}_\Gamma$ is given by

$$\{A, B\} = \delta A \circ G_C \circ \delta B .$$

(1.13)

Applied to the basic variable $\Phi^x$ — a value of the field at a point $x$, we get

$$\{\Phi^x, \Phi^y\} = G_{C}^{xy} .$$

(1.14)

The definitions of the symplectic structure and the causal Green function give us

$$\phi = - G_C \bullet \partial F[\Sigma] \bullet \phi = - G_C \bullet \tilde{dF}[\Sigma] \bullet \phi + G_C \bullet \hat{dF}[\Sigma] \bullet \phi$$

(1.15)

Using the fact that $\tilde{dF}[\Sigma]_{xy}$ as a function of $y$ has a support on $\Sigma_t$ and does not include any derivatives in directions out of $\Sigma$ and that

$$G_{C}^{xy} = 0 \quad \text{for} \quad x, y \in \Sigma ,$$

(1.16)

we see that the operator

$$D_\varphi[\Sigma] = - G_C \bullet \tilde{dF}[\Sigma]$$

(1.17)

plays a role of a projector on the subspace of solutions with zero normal derivative on $\Sigma$, and the operator

$$D_\pi[\Sigma] = G_C \bullet \hat{dF}[\Sigma]$$

(1.18)

is a projector on a subspace of solutions with zero value on $\Sigma$. Let’s summarize the properties of the operators $D_\varphi[\Sigma]$ and $D_\pi[\Sigma]$: 

$$
\begin{align*}
D_\varphi[\Sigma] \circ D_\varphi[\Sigma] &= D_\varphi[\Sigma] , & D_\pi[\Sigma] \circ D_\pi[\Sigma] &= D_\pi[\Sigma] , \\
D_\varphi[\Sigma] \circ D_\pi[\Sigma] &= D_\pi[\Sigma] \circ D_\varphi[\Sigma] = 0 , \\
D_\varphi[\Sigma] + D_\pi[\Sigma] &= D_C[\Sigma] .
\end{align*}
$$

(1.19)

We can map tensors $\tilde{dF}[\Sigma], \hat{dF}[\Sigma], D_\varphi[\Sigma], D_\pi[\Sigma]$ to spaces $\Gamma^k_\Sigma$ using the map $\iota[\Sigma]$. We will use the same symbols for the result. The definitions (1.17), (1.18) of $D_\varphi[\Sigma], D_\pi[\Sigma]$ and relations (1.19) can be rewritten as

$$
\begin{align*}
\partial F &= D_\varphi[\Sigma] \circ \partial F \circ D_\varphi[\Sigma] + D_\pi[\Sigma] \circ \partial F \circ D_\varphi[\Sigma] , \\
G_C &= D_\varphi[\Sigma] \circ G_C \circ D_\varphi[\Sigma] + D_\pi[\Sigma] \circ G_C \circ D_\varphi[\Sigma] , \\
\tilde{dF}[\Sigma] &= D_\pi[\Sigma] \circ \tilde{dF}[\Sigma] \circ D_\varphi[\Sigma] , & \hat{dF}[\Sigma] &= D_\varphi[\Sigma] \circ \hat{dF}[\Sigma] \circ D_\pi[\Sigma] .
\end{align*}
$$

(1.20) (1.21) (1.22)

We will also introduce the “inversions” of bi-forms $\tilde{dF}[\Sigma], \hat{dF}[\Sigma] \in H^0_2$

$$
\begin{align*}
\tilde{dF}[\Sigma]^{-1} \bullet \tilde{dF}[\Sigma] &= D_\pi[\Sigma] , & \hat{dF}[\Sigma] \bullet \hat{dF}[\Sigma]^{-1} &= D_\varphi[\Sigma] , \\
\tilde{dF}[\Sigma] \bullet \hat{dF}[\Sigma]^{-1} &= D_\pi[\Sigma] , & \hat{dF}[\Sigma]^{-1} \bullet \hat{dF}[\Sigma] &= D_\varphi[\Sigma]
\end{align*}
$$

(1.23)

and similarly for $\tilde{dF}[\Sigma], \hat{dF}[\Sigma] \in \Gamma^0_2$.

Using the covariant phase space $\Gamma$ and a solution $\Phi$ of Eq. (1.2) as a basic variable is nothing other than the “Heisenberg picture” in classical physics.
Quantization

Quantization is a heuristic procedure of construction of a quantum theory for a given classical theory. Let us have a classical system described by a phase space $\Gamma$ and symplectic structure $\partial F$. Observables are functions on $\Gamma$, and the Poisson bracket is given by (1.13). Quantization tells us to assign to at least some observables quantum observables — operators on a quantum Hilbert space $\mathcal{H}$. Let denote the space of operators $L(\mathcal{H})$. We will use letters with a hat to denote operators. The quantum observables should satisfy the same algebraic relations as the classical ones and commutation relations generated by Poisson brackets.

If the quantum versions of classical observables $A, B$ and $C = \{A, B\}$ are $\hat{A}, \hat{B}, \hat{C}$, they should satisfy

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -i\hat{C}.$$  (1.24)

It is well known that the procedure described above is not possible to carry out for all classical observables. Because quantum observables do not commute we have an “ordering problem” for observables given by a product of noncommuting observables.

For a scalar field we would like to define a quantum theory as the using basic observable $\Phi^x$ — a “value of field at point $x$”. Using Eq. (1.14) we can write the commutation relations for $\hat{\Phi}^x$ as

$$[\hat{\Phi}^x, \hat{\Phi}^y] = -i\hat{G}^{xy}_{C},$$  (1.25)

where $\hat{G}^{xy}_{C}$ is a quantum version of the causal Green function $G_C$. But for an interacting field $G_C$ does depend on $\Phi$ (position in $\Gamma$). This means that to define $\hat{G}^{xy}_{C} = G_C(\hat{\Phi})$ we have to solve the ordering problem. This is generally a nontrivial task.

This problem can be to solved for linear theories, for example, that of a free scalar field. In this case the causal Green function $G_C$ is constant on $\Gamma$ (independent of $\Phi$). Therefore its quantum version is proportional to the unit operator $\hat{1}$ (Poisson brackets of any observable with a constant are zero, so the quantum version of a constant observable has to commute with all observables). So

$$[\hat{\Phi}^x, \hat{\Phi}^y] = -iG_C^{xy} \hat{1}.$$  (1.26)

This means that we do not have any ordering problem in the quantization of observables $\Phi^x$. These observables are linear on $\Gamma$, and any linear observable can be generated from them without the multiplication of two noncommuting observables. So we have a unique quantization of all linear observables on the phase space $\Gamma$.

For quadratic observables

$$A(\Phi) = \frac{1}{2} \Phi \circ a \circ \Phi, \quad a \in \Gamma_2^0,$$  (1.27)

we have an ambiguity in the ordering of two $\hat{\Phi}$ observables. However, because the commutator of two $\hat{\Phi}$ is proportional to the unit operator, any quantum version of $A(\Phi)$ can be written as

$$\hat{A} = \frac{1}{2} \hat{\Phi} \circ a \circ \hat{\Phi} + \alpha \hat{1},$$  (1.28)

where the factor $\alpha$ is given by a particular choice of an operator ordering.

Infinite dimension of the phase space

We are working with $\Gamma$ and $\mathcal{H}$ on very formal level. More precisely using structures on $\Gamma$ and a quantization scheme, we define a quantum algebra of observables (generated by an algebra valued distribution $\hat{\Phi}$) which we want to represent using operators on $\mathcal{H}$. The representation is unique (up to unitary transformations) in the case of a finite dimensional phase space $\Gamma$. But there exist unitarily inequivalent representations of the quantum algebra on $\mathcal{H}$ in the case of a infinite dimensional phase space $\Gamma$. The phase space of the scalar field theory is infinite dimensional, and we really will deal with inequivalent representations.
We will adopt the following intuitive point of view. We will look on $\mathcal{H}$ as a vector space with a “quantum product” between any two states (vectors). However, there exist sets of states with a nondegenerated quantum product for any two states from the same set but maybe a degenerated quantum product for states from different sets. Each of these sets with restriction of the quantum product on it forms a Hilbert space, but there is no well defined unitary operator in this Hilbert space which relates one set to other set.

However it is useful keep all these sets together in one quantum space $\mathcal{H}$ with “generalized” quantum product. Intuitively these sets represents different “phases” of the same physical system. Physically a vacuum of one phase will contain an infinite mean number of particles of other phase.

For a complete discussion of inequivalent representation see \[7, 11\].

2 Particle interpretation

What are particles and why we need them?

In this part we would like to discuss quantization of the free scalar field in more detail. We have seen that the algebra of quantum observables is generated by basic observable $\hat{\Phi}$ with commutation relations (1.14), and we have a unique quantum version of any classical linear observable. For quantization of nonlinear observables we have to choose a particular operator ordering.

But we would like to find more about the structure of the space $\mathcal{H}$. For the interpretation of a theory we usually need to pick up quantities which are measurable in a physical experiment. This means one needs to find quantities to which a realistic detector coupled to the field is sensitive. But we need even more for understanding a theory. We would like to have an intuitive picture, a more descriptive way how to speak about our quantum system.

A very useful way to describe a quantum field is a language of particles. It is possible to construct special states representing “definite numbers of quanta of field”, and the structure of the theory becomes often much simpler when it is expressed in terms of these states. Particle states do not have to be always straightforwardly measurable quantities — only in special situations it is possible to construct a simple detector sensitive exactly to some particle states. But even in situations when it is not simple to prepare the system in a particle state, it can be useful to use such states for description of physical processes.

First we have to define what particles are. Here is a short list of some elementary properties of particles:

- discrete nature of particles
- particles as quanta of energy
- definiteness of position or momenta of particles
- measurability by a detector
- a connection with quantization of a relativistic particle

The first property is the property we will use the most. Particles can be counted; they have a piece-like character. We speak about photons because we are able to detect discrete hits on a screen when we illuminate it by a weak electromagnetic field. We speak about quanta of energy in the case of a hydrogen atom because the atom can emit the energy in discrete pieces.

A discrete nature is only one of many properties of classical particles. But we are not speaking about classical particles. We want to construct a useful notion of particles for quantum field theory. And the notion of discrete pieces gives us the weakest sense of the word particle. Or, maybe, it would be better to speak about quanta of the field.

Of course, we can be more restrictive about the notion of particles. As the second item in our list suggests, we could require that particles are quanta of energy - i.e. that some particle states are eigenstates of a Hamiltonian of our system. We will discuss this condition later. Let us only say that this condition picks up a unique notion of particles but, unfortunately, in a general situation we do not have a unique notion of energy.
Similarly, it is difficult to give a well defined sense to position or momentum of a particle in a general spacetime. Only in the case when our spacetime is sufficiently special we can introduce some generalized momentum operator or to find a simple detector sensitive exactly to some kind of particles [4,12]. Localizability is an even more subtle issue.

There exists a complete different way how to construct quantum field theory [3, 13, 14]. It is possible to quantize a relativistic particle using a sum over histories approach and to find that transition amplitudes calculated in this way are exactly the same as amplitudes between some particle states of the scalar field theory [14]. It gives us another interesting meaning to particle states.

**Fock structure of the quantum space \( \mathcal{H} \).**

Now let us concentrate on the basic particle property — the discrete nature of particles. We would like to speak about a state with no particles, about states with one particle, two particles and so on. The representation of this structure in quantum mechanics is well known. We want to find a Fock structure in our quantum space \( \mathcal{H} \) which divides \( \mathcal{H} \) to subspaces with a vacuum state, one, two and more particle states. As known, the Fock structure can be generated by creation and annihilation operators \( \hat{a}_k^\dagger \) and \( \hat{a}_k \) which satisfy the commutation relations

\[
[\hat{a}_k, \hat{a}_l] = 0 \ , \quad [\hat{a}_k^\dagger, \hat{a}_k^\dagger] = 0 \ , \quad [\hat{a}_k, \hat{a}_l^\dagger] = \alpha_{kl} \hat{1} \ ,
\]

where indexes \( k, l \) label one-particle states and \( \alpha_{kl} \) is a transition amplitude between two one-particle states labeled by \( k \) and \( l \). So, to find a particle interpretation of the free scalar field theory we need to construct such creation and annihilation operators from our basic observable \( \Phi \). The construction which we will describe below is possible to find in \( [2] \).

First we describe a way in which we will label one-particle states. Particles used for the description of a scalar field are scalar particles without any inner degrees of freedom. This means that on the classical level the position and momenta at one time are sufficient for the determination of the state of one particle. Therefore the quantum space \( \mathcal{H}_1 \) of one-particle states should be “\( \infty^3 \)” dimensional (one vector of a base for each space point) as a complex vector space (let’s denote it \( \mathbb{C} \)-dimensionality). It means that as real vector space it has “the same” \( \mathbb{R} \)-dimension as the phase space \( \Gamma \) of the scalar field — “\( 2\infty^3 \)”. These formal consideration suggest the use of the space \( \Gamma \) for labeling of one-particle states. More precisely, we would like to find a one-to-one map between spaces \( \mathcal{H}_1 \) and \( \Gamma \).

This faces us with a problem. Some vectors in \( \mathcal{H}_1 \) are related only by a phase and essentially represent the same physical state. But their images (labels) in \( \Gamma \) are different. We would like to know how these different labels are related. This means that we need to introduce a structure of a Hilbert space to the phase space \( \Gamma \) in such way that our mapping between \( \Gamma \) and \( \mathcal{H}_1 \) will be an isomorphism of Hilbert spaces.

For this we need to speak about \( \Gamma \) as a complex vector space with a positive definite scalar product. Therefore we need to define “a multiplication by a complex number” in \( \Gamma \). We do not want to complexify \( \Gamma \) to \( \Gamma^C = \mathbb{C} \otimes \Gamma \) because it would “doubled” the dimension. We need a multiplication by a complex number inside of \( \Gamma \).

To do it, it is sufficient to define multiplication by an imaginary unity. Let define for \( \phi \in \Gamma \)

\[
i \star \phi = J \circ \phi \ ,
\]

where “\( \star \)” represents multiplication of a vector from \( \Gamma \) by a complex number which we are defining and \( J \) is an operator on \( \Gamma \). It is clear that for consistency \( J \) has to be a linear operator (it is already reflected in using “\( \circ \)” operation) which satisfies

\[
J \circ J = -\delta \ .
\]

Such operator is called a complex structure on the vector space \( \Gamma \). There exist a lot of different complex structures on \( \Gamma \), and we will discuss their relation in part \( [2] \). At this moment we will pick up one which we denote \( J_p \), and we will use the index \( p \) for all quantities which depend on this complex structure.
Next we need to define a positive definite product on $\Gamma$. It is possible to do if we will assume that $J_p$ possess the following properties

$$J_p \circ \partial F \circ J_p = \partial F \quad \Leftrightarrow \quad J_p \circ \partial F = -\partial F \circ J_p ,$$

$$\gamma_p = J_p \circ \partial F \quad \text{is positive definite} .$$

The first property is called compatibility of $J_p$ with the symplectic structure $\partial F$. Let’s note that if $J_p$ is compatible with $\partial F$, the bi-form $\gamma_p$ is automatically symmetric. Let assume that $J_p$ satisfies both conditions (2.4) and (2.5). Now we can define a scalar product on $\Gamma$ by

$$\langle \phi_1, \phi_2 \rangle_p = \phi_1 \circ \frac{1}{2}(\gamma_p - i\partial F) \circ \phi_2 .$$

It is linear in the second argument, antilinear in the first one and positive definite.

$$\langle i \ast \phi_1, \phi_2 \rangle_p = -i\langle \phi_1, \phi_2 \rangle_p \quad , \quad \langle \phi_1, i \ast \phi_2 \rangle_p = i\langle \phi_1, \phi_2 \rangle_p ,$$

$$\langle \phi, \phi \rangle_p = \frac{1}{2} \phi \circ \gamma_p \circ \phi > 0 \quad \text{for} \quad \phi \neq 0 .$$

We finally changed the phase space $\Gamma$ to a Hilbert space $\Gamma_p = (\Gamma, \ast, (, )_p)$ using a new extra structure $J_p$. Now we can proceed and define creation and annihilation operators acting on $H$ which are labeled by vectors from $\Gamma$:

$$\hat{a}_p[\phi] = \langle \phi, \hat{\Phi} \rangle_p \quad , \quad \hat{a}_p[\phi]^\dagger = \langle \hat{\Phi}, \phi \rangle_p$$

for any $\phi \in \Gamma$. We will show below (see Eq. [2.31]) that the commutation relations of such defined operators are

$$[\hat{a}_p[\phi_1], \hat{a}_p[\phi_2]] = 0 \quad , \quad [\hat{a}_p[\phi_1]^\dagger, \hat{a}_p[\phi_2]^\dagger] = 0 ,$$

$$[\hat{a}_p[\phi_1], \hat{a}_p[\phi_2]^\dagger] = \langle \phi_1, \phi_2 \rangle_p \hat{1} \quad .$$

We see that they really satisfy the commutation relations of creation and annihilation operators. We can define a vacuum state by the condition

$$\hat{a}_p[\phi]|p : \text{vac}\rangle = 0 \quad \text{for each} \quad \phi \in \Gamma \quad ,$$

$$\langle p : \text{vac}|p : \text{vac}\rangle = 1$$

and multiple particle states by

$$\hat{a}_p[\phi_1]^\dagger \hat{a}_p[\phi_2]^\dagger \ldots |p : \text{vac}\rangle \quad .$$

The mapping between the phase space $\Gamma_p$ and the one-particle space $H_1$ is given by

$$\phi \quad \leftrightarrow \quad \hat{a}_p[\phi]^\dagger |p : \text{vac}\rangle$$

and is really an isomorphism of Hilbert spaces

$$\langle p : \text{vac}|\hat{a}_p[\phi_1]^\dagger \hat{a}_p[\phi_2]^\dagger |p : \text{vac}\rangle = \langle p : \text{vac}|\hat{a}_p[\phi_1], \hat{a}_p[\phi_2]^\dagger |p : \text{vac}\rangle = \langle \phi_1, \phi_2 \rangle_p \quad ,$$

$$i \ast \phi \quad \leftrightarrow \quad \hat{a}_p[i \ast \phi]^\dagger |p : \text{vac}\rangle = i\hat{a}_p[\phi]^\dagger |p : \text{vac}\rangle .$$

We have successfully found a Fock structure in our quantum space $H$ with one-particle states labeled by vectors from the classical phase space of the scalar field $\Gamma$. We will call such construction a \textit{particle interpretation} of the scalar field theory. For this construction we have used a new element — the complex structure $J_p$. We can expect that different complex structures can give us different Fock structures in $H$, and we will investigate this question in part 3.
We also implicitly assumed that condition (2.11) selects a unique vacuum state (up to a phase) and creation operators acting on the vacuum state generate a complete set of vectors in $\mathcal{H}$. This assumption corresponds to the assumption that the set of observables $\Phi^x$ for $x \in M$ is a sufficient set of observables for description of our system, i.e. that we do not have any other degrees of freedom which are not reflected in field observables $\Phi^x$. In the opposite case we should use another kind of field.

From the strict mathematical point of view we have constructed a particular representation of the quantum algebra of observables generated by $\Phi^x$ on a Fock space based on one-particle space isomorphic with $\Gamma_p$.

**Positive-negative frequency splitting**

Now we will show a connection with the usual definition of particle states using a mode expansion of the field operator [4]. For it we have to investigate properties of the complex structure. $J_p$ as an operator on $\Gamma$ does not have eigenvectors in $\Gamma$, but it has eigenvectors in the complexification $\Gamma^C = \mathbb{C} \otimes \Gamma$ of the phase space. Its eigenvalues are $\pm i$ (because squares of them have to be $-1$) and we can explicitly write projectors on subspaces of $\Gamma^C$ with these eigenvalues

$$P^\pm_p = \frac{1}{2} (\delta \mp i J_p) \quad .$$

They have properties

$$J_p \circ P^+_p = i P^+_p \quad , \quad J_p \circ P^-_p = -i P^-_p \quad ,$$

$$P^\pm_p \circ P^\mp_p = P^\pm_p \quad , \quad P^\pm_p \circ P^\mp_p = 0 \quad , \quad P^\pm_p \circ P^\mp_p = P^\mp_p \quad ,$$

$$P^+_p + P^-_p = \delta \quad , \quad i(P^+_p - P^-_p) = J_p \quad .$$

The compatibility (2.4) of $J_p$ and $\partial F$ is possible to reformulate as

$$P^\pm_p \circ \partial F \circ P^\mp_p = 0 \quad , \quad \partial F = P^-_p \circ \partial F \circ P^+_p + P^+_p \circ \partial F \circ P^-_p \quad .$$

$$P^\pm_p \circ \gamma_p \circ P^\mp_p = 0 \quad , \quad \partial F = P^-_p \circ \gamma_p \circ P^+_p + P^+_p \circ \gamma_p \circ P^-_p \quad ,$$

$$P^\pm_p \circ G_C \circ P^\mp_p = 0 \quad , \quad G_C = P^-_p \circ G_C \circ P^+_p + P^+_p \circ G_C \circ P^-_p \quad .$$

We will call the positive resp. negative frequency part of a solution $\phi$ of the equation of motion (1.3) (i.e. $\phi \in \Gamma$) the complex solutions $\phi^+_p$ resp. $\phi^-_p$ of the same equation (i.e. $\phi^+_p \in \Gamma^C$) defined by

$$\phi^\pm_p = P^\pm_p \circ \phi \quad .$$

We have

$$\phi = \phi^+_p + \phi^-_p \quad , \quad J_p \circ \phi = i(\phi^+_p - \phi^-_p) \quad , \quad \phi^+_p \circ \phi^-_p = \phi^+_p \quad .$$

The scalar product is possible to write as

$$\langle \phi_1, \phi_2 \rangle_p = \phi^+_1 \circ \gamma_p \circ \phi^+_2 = -i \phi^-_1 \circ \partial F \circ \phi^+_2 \quad .$$

We see that the scalar product $\langle \phi_1, \phi_2 \rangle_p$ is essentially the Klein-Gordon product of the negative and positive frequency parts of $\phi_1$ and $\phi_2$.

Let’s note that not all linear operators on $\Gamma$ are also $p$-linear on $\Gamma_p$. $p$-linearity of an operator $L$ means that $L$ is linear with respect of multiplication $\ast$. Therefore it has to commute with multiplication by imaginary unity which is given by action of the complex structure $J_p$, i.e.

$$L \circ J_p = J_p \circ L \quad .$$

(2.24)
Similarly $p$-antilinearity of an operator $A$ is equivalent to
\[ A \circ J_p = -J_p \circ A \quad . \quad (2.25) \]

We introduce the hermitian conjugation $L^{(t)}$ of a $p$-linear operator $L$ defined by
\[ \langle \phi_1 \circ L^{(t)}, \phi_2 \rangle_p = \langle \phi_1, L \circ \phi_2 \rangle_p \quad , \quad L^{(t)} = -G_C \circ L \circ \partial F \quad . \quad (2.26) \]

We see that it depends on the choice of $J_p$ only through the $p$-linearity condition on $L$. Similarly we can define “transposition” $A^{(T)}$ for a $p$-antilinear operator $A$
\[ \langle \phi_1 \circ A^{(T)}, \phi_2 \rangle_p^* = \langle \phi_1, A \circ \phi_2 \rangle_p \quad , \quad A^{(T)} = G_C \circ A \circ \partial F \quad . \quad (2.27) \]

Both these operator are particular cases of the transposition $O^{Tr}$ of any operator $O$ on $\Gamma$ defined using the bi-form $\gamma_p$:
\[ O^{Tr} = \gamma_p^{-1} \circ O \circ \gamma_p \quad , \quad (2.28) \]
\[ L^{(t)} = L^{Tr} \quad , \quad A^{(T)} = A^{Tr} \quad . \quad (2.29) \]

This operation depends on the choice of $J_p$ explicitly.

We can also express creation and annihilation operators using $P^\pm_p$
\[ \hat{a}[\phi] = -i \phi^- \circ \partial F \circ \hat{\Phi} = -i \phi \circ \partial F \circ \hat{\Phi}^+ \quad , \quad (2.30) \]
\[ \hat{a}[\phi]^\dagger = i \phi^+ \circ \partial F \circ \hat{\Phi} = i \phi \circ \partial F \circ \hat{\Phi}^- \quad . \]

It means that positive resp. negative frequency part of the field operator $\hat{\Phi}$ is composed only from annihilation resp. creation operators and vice versa. Using these expressions we can easily prove the commutation relations (2.31). For example,
\[ [\hat{a}[\phi], \hat{a}[\phi]^\dagger] = -i \phi \circ P^- \circ \partial F \circ \hat{\Phi} \circ \partial F \circ P^+ \circ \phi 2 i = \]
\[ = \phi \circ P^- \circ \partial F \circ iG_C \circ \partial F \circ P^+ \circ \phi 2 \hat{1} = -i \phi \circ P^- \circ \partial F \circ P^+ \circ \phi 2 \hat{1} \quad = \quad (2.31) \]
\[ = \langle \phi_1, \phi_2 \rangle_p^* \hat{1} \quad . \]

Now we can choose a $p$-orthonormal $\mathbb{C}$-base $u = \{ u_k; k \in \mathcal{I} \}$ in $\Gamma_p$ where $k$ is an index from some, for simplicity discrete, set $\mathcal{I}$. $p$-orthonormality means
\[ \langle u_k, u_l \rangle_p = \delta_{kl} \quad . \quad (2.32) \]

$\mathbb{C}$-base means that the set $u$ is complete in the Hilbert space $\Gamma_p$, i.e. in the vector space with multiplication $\star$. The set $\{ u_{kp}^+, u_{kp}^-; k \in \mathcal{I} \}$ of positive and negative frequency parts of vectors $u_k$ forms a complete set in $\Gamma^\mathbb{C}$ with properties
\[ u_{kp}^\pm \circ \partial F \circ u_{kp}^\pm = 0 \quad , \quad -iu_{kp}^- \circ \partial F \circ u_{kp}^+ = \delta_{kl} \quad , \quad (2.33) \]
\[ u_{kp}^\pm \star = u_{kp}^\mp, \quad F \star u_{kp}^\pm = 0 \quad . \]

These are standard properties of modes which are used for the expansion of a field operator. We can decompose $\hat{\Phi} \in \Gamma \otimes L(\mathcal{H})$ using the base $\{ u_{kp}^+, u_{kp}^-; k \in \mathcal{I} \}$
\[ \hat{\Phi} = \sum_{k \in \mathcal{I}} (\hat{a}_k u_{kp}^+ + \hat{a}_k^\dagger u_{kp}^-) \quad , \quad (2.34) \]

where operator valued coefficients can be found using the relations (2.33)
\[ \hat{a}_k = -i u_{kp}^- \circ \partial F \circ \hat{\Phi} = \hat{a}_p[u_k] \quad , \quad (2.35) \]
\[ \hat{a}_k^\dagger = -i \hat{\Phi} \circ \partial F \circ u_{kp}^+ = \hat{a}_p[u_k]^\dagger \quad . \]

We see that the usual mode expansion gives nothing other than our creation and annihilation operators for a chosen base $u$ in the phase space $\Gamma$. This connection also justifies using the words “positive” resp. “negative frequency part” for vectors from $P^\pm_p \circ \Gamma$. 

10
Green functions

We can ask whether the construction of the Fock structure in $\mathcal{H}$ using the complex structure is not artificial. Does $J_p$ have any physical meaning? Is it connected with any interesting physical quantity? The answer is yes. The complex structure has a rather simple interpretation. To show it we have to introduce Green functions associated with a particular choice of vacuum state.

The Wightman functions are defined by

$$G^+_p = \langle p : vac|\hat{\Phi}^x\hat{\Phi}^y|p : vac \rangle \quad , \quad G^-_p = \langle p : vac|\hat{\Phi}^y\hat{\Phi}^x|p : vac \rangle \quad . \quad (2.36)$$

The Hadamard Green function is

$$G^{(1)}_p = \langle p : vac|\hat{\Phi}^x\hat{\Phi}^y + \hat{\Phi}^y\hat{\Phi}^x|p : vac \rangle \quad . \quad (2.37)$$

The causal Green function can be written as

$$-iG^C_{xy} = \langle p : vac|\hat{\Phi}^x\hat{\Phi}^y - \hat{\Phi}^y\hat{\Phi}^x|p : vac \rangle \quad . \quad (2.38)$$

All these Green functions are solution of the equation of motion (1.2) in both arguments and therefore they are bi-vectors from $\Gamma^2_{0,2}$.

We can also define the Feynman Green function

$$G^F_{xy} = \langle p : vac|T(\hat{\Phi}^x\hat{\Phi}^y)|p : vac \rangle \quad , \quad (2.39)$$

where $T$ denotes time ordering of operators

$$T(\hat{\Phi}^x\hat{\Phi}^y) = \begin{cases} 
\hat{\Phi}^x\hat{\Phi}^y & \text{for } x \text{ after } y \\
\hat{\Phi}^y\hat{\Phi}^x & \text{for } y \text{ after } x 
\end{cases} \quad . \quad (2.40)$$

For $x, y$ space-like separated $\hat{\Phi}^x$ and $\hat{\Phi}^y$ commute, so the definition is unique. Finally we define retarded, advanced and symmetric Green functions

$$(\chi[\Omega] \delta) \bullet F \bullet G_{ret,adv} = - (\chi[\Omega] \delta) \quad \text{for any } \Omega = \langle \Sigma_f | \Sigma_i \rangle \quad , \quad (2.41)$$

$$G_{ret} = 0 \quad \text{for } x \text{ before } y \quad , \quad G_{adv} = 0 \quad \text{for } x \text{ after } y \quad , \quad (2.41)$$

$$\bar{G} = \frac{1}{2}(G_{ret} + G_{adv}) \quad . \quad (2.42)$$

Relations among these Green functions are

$$G^{(1)}_p = G^+_p + G^-_p \quad , \quad G_C = i(G^+_p - G^-_p) \quad , \quad (2.43)$$

$$G^+ = \frac{1}{2}(G^{(1)}_p - iG_C) \quad , \quad G^+ = \frac{1}{2}(G^{(1)}_p + iG_C) \quad , \quad (2.44)$$

$$G^+_p = G^+_p \quad , \quad G^{(1)}_p = G^{(1)}_p \quad , \quad G^F = G^F \quad , \quad G^C = -G_C \quad , \quad (2.45)$$

$$G^{+\ast}_p = G^-_p \quad , \quad G^{(1)\ast}_p = G^{(1)}_p \quad , \quad G^F = G^F \quad , \quad G^C = G_C \quad , \quad (2.46)$$

$$G_C = G_{ret} - G_{adv} \quad , \quad \bar{G} = \frac{1}{2}(G_{ret} + G_{adv}) \quad , \quad (2.47)$$

$$G^F_{xy} = \begin{cases} 
G^+_p & \text{for } x \text{ after } y \\
G^-_p & \text{for } x \text{ before } y \\
G^+_p = G^-_p = \frac{1}{2}G^{(1)}_p & \text{for } x, y \text{ space-like separated }
\end{cases} \quad . \quad (2.48)$$
Using these relations we can derive
\[ G^F_p = -i\hat{G} + \frac{1}{2} G^{(1)}_p \] (2.49)
and therefore the Feynman Green function satisfies
\[ -i(\chi[\Omega]\delta) \bullet F \bullet G^F_p = (\chi[\Omega]\delta) \quad \text{for any} \quad \Omega = \langle \Sigma_f | \Sigma_i \rangle. \] (2.50)

This means that Green functions \( G^F_p, G_{ret}, G_{adv}, \tilde{G} \) are not tensors from \( \Gamma_0^2 \) but rather they belong to \( H_0^2 \).

Let’s note that Green functions \( G_{ret}, G_{adv}, \tilde{G} \) are independent on the choice of the complex structure \( J_p \). Green functions \( G^+_p, G^-_p, G^{(1)}_p \) and \( G^F_p \) depend on the choice of vacuum state and therefore on the choice of the particle interpretation.

After introducing this whole zoo of Green functions we will pay more attention to \( G^+_p, G^-_p \) and \( G^{(1)}_p \). Using the fact that the positive frequency part of \( \hat{\Phi} \) annihilates the vacuum state we get
\[ P^+_p \circ G^+_p \circ \partial F = \pm i G^+_p \circ \partial F \] (2.51)
and
\[ P^-_p \circ G^-_p \circ \partial F = 0 \] (2.52)
\[ G^{(1)}_p = -i (P^+_p - P^-_p) \circ G_C = -J_p \circ G_C = \gamma_p^{-1} \] (2.53)

This means that the complex structure \( J_p \) is essentially the Hadamard Green function. Or, more precisely, the action of \( J_p \) on a solution \( \phi \in \Gamma \) is given by Klein-Gordon product of the Hadamard Green function with the solution \( \phi \). Wightman functions are in similar relations with projector operators \( P^\pm_p \).

We can use this relation to derive compositions laws for Green functions. The translation of equations (2.17), (2.3) to the language of Green functions gives us
\[ G^\pm_p \circ \partial F \circ G^\pm_p = \pm i G^\pm_p \] (2.54)
\[ G^{(1)}_p \circ \partial F \circ G^{(1)}_p = G_C \] (2.55)

Using (2.48) we get
\[ (\chi[\Omega_f]\delta) \bullet G^F_p \bullet \partial F[\Sigma] \bullet G^F_p \bullet (\chi[\Omega_i]\delta) = i (\chi[\Omega_f]\delta) \bullet G^F_p \bullet (\chi[\Omega_i]\delta) \] (2.56)
for any Cauchy hypersurface \( \Sigma \) and spacetime domains \( \Omega_f \) resp. \( \Omega_i \) in the future resp. the past of the hypersurface \( \Sigma \).

**Total particle-number observable**

We can define a quantum observable of the number of particles in a state labeled by a solution \( \phi \)
\[ \hat{n}_p[\phi] = \frac{\hat{a}_p[\phi] \hat{a}_p[\phi]}{\langle \phi, \phi \rangle_p}. \] (2.59)

It satisfies
\[ \hat{n}_p[\phi] \hat{a}_p[\phi]^\dagger m|p : vac\rangle = m \hat{a}_p[\phi]^\dagger m|p : vac\rangle. \] (2.60)
Let's choose again a p-orthonormal \( \mathbb{C} \)-base \( u = \{ u_k; k \in I \} \) in \( \Gamma_p \). It generates an orthonormal base in quantum space \( \mathcal{H} \) composed of particle states

\[
|p \ u : m \rangle = \frac{1}{\sqrt{m!}} \hat{a}(u)^m |p : \text{vac}\rangle.
\] (2.61)

Here \( m = \{ m_k; k \in I \} \) is a multiindex and we are using shorthands

\[
m! = \prod_{k \in I} m_k!, \quad \hat{a}(u)^m = \prod_{k \in I} \hat{a}(u_k)^{m_k},
\] (2.62)

where creation operators \( \hat{a}(u)^m \) are defined by Eq. (2.35). The combinatoric factor is chosen so that states are normalized:

\[
\langle p \ u : m | p \ u : m' \rangle = \delta_{mm'}.
\] (2.63)

The observable of the number of particles in a mode \( u_k \) is

\[
\hat{n}_p u_k = \hat{n}_p[u_k] = \hat{a}_k^\dagger \hat{a}_k,
\] (2.64)

and it satisfies

\[
\hat{n}_p u_k |p \ u : m \rangle = m_k |p \ u : m \rangle.
\] (2.65)

Now we can define the observable of the total number of \( p \)-particles

\[
\hat{N}_p = \sum_{k \in I} \hat{n}_p u_k.
\] (2.66)

Using definitions (2.33) of creation and annihilation operators and orthonormality of the base \( u \) we get

\[
\hat{N}_p = \sum_{k \in I} \hat{a}_p[u_k] \hat{a}_p[u_k] = \sum_{k \in I} \langle \hat{\Phi}, u_k \rangle_p \langle u_k, \hat{\Phi} \rangle_p = \langle \hat{\Phi}, \hat{\Phi} \rangle_p.
\] (2.67)

We see that \( \hat{N}_p \) is independent on the choice of the base \( u \) but it depends on the complex structure \( J_p \) through the scalar product and therefore it depends on the particle interpretation. It will be useful to write down also another representation of \( \hat{N}_p \). First let's note

\[
\hat{\Phi} \circ \partial F \circ \hat{\Phi} = -i \left( \frac{1}{2} \text{tr}_{\Gamma_p} \delta^{(\Gamma_p)} \right) \hat{\Phi} = -i \left( \text{tr}_{\Gamma_p} \delta^{(\Gamma_p)} \right) \hat{\Phi}.
\] (2.68)

So

\[
\hat{N}_p = \langle \hat{\Phi}, \hat{\Phi} \rangle_p = \frac{1}{2} \hat{\Phi} \circ (\gamma_p - i \partial F) \circ \hat{\Phi} = \frac{1}{2} \hat{\Phi} \circ \gamma_p \circ \hat{\Phi} - \frac{1}{2} \left( \text{tr}_{\Gamma_p} \delta^{(\Gamma_p)} \right) \hat{\Phi}.
\] (2.69)

We see that \( \hat{N}_p \) is a quantum version of a classical quadratic observable

\[
N_p = \frac{1}{2} \Phi \circ \gamma_p \circ \Phi
\] (2.70)

with special operator ordering. This operator ordering is called \( p \)-normal ordering and is defined by the condition that in any product of operators all \( p \)-creation operators are on the left of all \( p \)-annihilation operators. We denote a quantum version of a classical observable \( F(\Phi) \) in \( p \)-normal ordering by

\[
\hat{F} = :F(\hat{\Phi})_p.\] (2.71)
It can be written more explicitly for any quadratic observable defined using a symmetric bi-form $k \in \Gamma^0_2$

$$K(\Phi) = \frac{1}{2} \Phi \circ k \circ \Phi = \frac{1}{2} (\Phi^+_p + \Phi^-_p) \circ k \circ (\Phi^+_p + \Phi^-_p) =$$

$$= \frac{1}{2} \Phi^+_p \circ k \circ \Phi^+_p + \frac{1}{2} \Phi^-_p \circ k \circ \Phi^-_p + \Phi^-_p \circ k \circ \Phi^+_p , \quad (2.72)$$

$$\hat{K} = :K(\hat{\Phi});_p = \frac{1}{2} \hat{\Phi}^+_p \circ k \circ \hat{\Phi}^+_p + \frac{1}{2} \hat{\Phi}^-_p \circ k \circ \hat{\Phi}^-_p + \hat{\Phi}^-_p \circ k \circ \hat{\Phi}^+_p . \quad (2.73)$$

For the observable $N_p(\Phi)$ using Eq. (2.19) we get

$$\hat{N}_p = \hat{\Phi}^-_p \circ \gamma_p \circ \hat{\Phi}^+_p = :N_p(\hat{\Phi});_p \quad . \quad (2.74)$$

**Diagonalization of Hamiltonian**

Let’s assume that a classical quadratic positive definite Hamiltonian is given,

$$H(\Phi) = \frac{1}{2} \Phi \circ h \circ \Phi , \quad (2.75)$$

where $h$ is a positive definite symmetric bi-form from $\Gamma^0_2$. We can ask whether there exists a particle interpretation such that particle states have definite energy and the energy is additive with respect to the number of particles. More precisely, we will look for such a complex structure $J_p$ and $p$-orthonormal base $u = \{u_k; k \in I\}$ which satisfy

$$\hat{H} \mid p u : m \rangle = \left( \sum_{k \in I} \omega_k m_k \right) \mid p u : m \rangle \quad , \quad (2.76)$$

where $\omega_k \in \mathbb{R}^+$ is the energy of the one-particle state $\hat{a}^+_k \mid p : vac \rangle$

$$\hat{H} \hat{a}^+_k \mid p : vac \rangle = \omega_k \hat{a}^+_k \mid p : vac \rangle \quad . \quad (2.77)$$

This requirement is equivalent to the requirement that the Hamiltonian have the form

$$\hat{H} = \sum_{k \in I} \omega_k \hat{n}_{p,k} \quad . \quad (2.78)$$

Using the definition of $\hat{n}_{p,k}$ (2.64) and the orthonormality of the base $u$, we get

$$\hat{H} = \sum_{k \in I} \langle \hat{\Phi},u_k \rangle_p \omega_k \langle u_k,\hat{\Phi} \rangle_p = \langle \hat{\Phi},\Omega \circ \hat{\Phi} \rangle_p = :\hat{\Phi} \circ \gamma_p \circ \Omega \circ \hat{\Phi} ;_p \quad , \quad (2.79)$$

where $\Omega$ is a $p$-linear hermitian positive definite operator on $\Gamma_p$ given by

$$\Omega \circ u_k = \omega_k u_k \quad . \quad (2.80)$$

$p$-linearity gives us the condition

$$[\Omega, J_p] = 0 \quad . \quad (2.81)$$

Hermiticity $\Omega^{(\dagger)} = \Omega$ (following from $\omega_k \in \mathbb{R}^+$) gives

$$\partial F \circ \Omega = \Omega \circ \partial F \iff \gamma_p \circ \Omega = \Omega \circ \gamma_p \quad . \quad (2.82)$$
The quantum observable \( \hat{H} \) should be a quantum version of the classical observable \( H(\Phi) \) in some operator ordering. As we have discussed, any two quantum versions of \( H(\Phi) \) defined using two different operator orderings can differ only by multiple of the unit operator. Therefore we can write

\[
\hat{H} = \hat{H}(\Phi) + \alpha \mathbb{1} = \hat{\Phi} \circ h \circ \hat{\Phi} + \alpha \mathbb{1} .
\]

From a comparison with Eq. (2.79) we see that we need to satisfy

\[
h = \gamma p \circ \Omega \iff G_C \circ h = J_p \circ \Omega .
\]

Let’s summarize. We are looking for a complex structure \( J_p \) and a positive definite operator \( \Omega \) which satisfy conditions (2.4), (2.5), (2.81), (2.82) and (2.84). We can get such a \( J_p \) and \( \Omega \) using a polar decomposition of the operator \( (G_C \circ h) \). For a polar decomposition we need a transposition of operators. Let us use the transposition defined using a positive definite symmetric bi-form

\[
A^T = h^{-1} \circ A \circ h \quad \text{for any operator } A \text{ on } \Gamma .
\]

Because \( G_C \circ h \) is antisymmetric with respect of this transposition, left and right polar decompositions of \( (G_C \circ h) \) coincide and we can define

\[
\Omega = |G_C \circ h| = ((G_C \circ h)^T \circ (G_C \circ h))^\frac{1}{2} = ((G_C \circ h) \circ (G_C \circ h)^T)^\frac{1}{2} ,
\]

\[
J_p = \text{sign}(G_C \circ h) = (G_C \circ h) \circ \Omega^{-1} = \Omega^{-1} \circ (G_C \circ h) ,
\]

\[
G_C \circ h = J_p \circ \Omega = \Omega \circ J_p .
\]

It is straightforward to check all conditions on \( J_p \) and \( \Omega \). Positive definiteness and symmetry \( (\Omega^T = \Omega) \) of \( \Omega \) follows from the definition of square root, the compatibility of \( J_p \) and \( \partial F \) follows from Eq. (2.87) and symmetry of \( \Omega \), positive definiteness of \( \gamma_p \) follows from Eq. (2.87) and positive definiteness of \( \Omega \), (2.81) and (2.84) are the same as Eq. (2.88).

We have finally proved that the positive quadratic classical Hamiltonian \( H(\Phi) \) picks up uniquely the particle interpretation in which it is possible to diagonalize the quantum Hamiltonian, i.e. to write

\[
\hat{H} = \hat{H}(\Phi) + \sum_{k \in I} \omega_k \hat{n}_{p, k} ,
\]

where \( \hat{n}_{p, k} \) are observables of number of particle in modes \( u_k \) which are eigenvectors of the operator \( \Omega \) with eigenvalues \( \omega_k \). A similar result is possible to find in \( \mathbb{I} \).

Unfortunately we do not have a preferable 3+1 splitting in a general spacetime, and for a general 3+1 splitting the Hamiltonian is time dependent. This means that the diagonalization criterion picks up different particle interpretations at different times. This reflects the fact that in a general spacetime we do not have a preferable particle interpretation and if we decide to choose particle interpretations connected with the Hamiltonian of some 3+1 decomposition, we have to expect particle creation as it will be described in part 3.

**Boundary conditions**

We have seen that Green functions \( G_p^+, G_p^{(1)}, G_p^F \) are associated with each particle interpretation. The Green functions of the same kind for different particle interpretations satisfy the same equations and symmetry conditions. They differ by boundary conditions. Now we will find what boundary conditions are associated with a particle interpretation.

First we will reformulate structures we have introduced earlier in the language of quantities localized on a hypersurface \( \Sigma \). Space field quantities are tensors from subspaces of \( H^k_\Sigma \) or \( \Gamma^k_\Sigma \) defined using the projector operator \( D_\Sigma[\Sigma] \). Therefore we need to express quantities as \( J_p, P^}_p \) using objects from these subspaces. But a general tensor from \( H^k_\Sigma \) or from \( \Gamma^k_\Sigma \) has also components in subspaces which are generated by the projector

15
For brevity of notation we drop the explicit dependence on $\Sigma$.

So we can write

$$D_p = A_p - B_p \circ D \hat{F} + dF^{-1} \circ C_p + dF^{-1} \circ D_p \circ dF,$$

where

$$A_p, D_p \in \Gamma^1 \ , \ B_p \in \Gamma^2 \ , \ C_p \in \Gamma^1 \ ,$$

$$A_p \circ D_p = D_p \circ A_p = 0 \ , \ D_p \circ D_p = D_p \circ D_p = 0 \ ,$$

$$B_p \circ D_p = D_p \circ B_p = 0 \ , \ C_p \circ D_p = D_p \circ C_p = 0 \ .$$

For brevity of notation we drop the explicit dependence on $\Sigma$.

The conditions (2.3), (2.4) give

$$D_p = -A_p \ , \ C_p = C_p^T \ , \ B_p = B_p^T \ ,$$

$$A_p \circ B_p = B_p \circ A_p \ , \ A_p \circ C_p = C_p \circ A_p \ ,$$

$$B_p \circ C_p = C_p \circ B_p = D_p + A_p \circ A_p \ .$$

So we can write

$$J_p = A_p - B_p \circ dF + dF^{-1} \circ C_p - dF^{-1} \circ A_p \circ dF \ ,$$

$$\gamma_p = C_p - dF \circ A_p - A_p \circ dF^{-1} - dF \circ B_p \circ dF \ ,$$

$$G_p^{(1)} = B_p + dF^{-1} \circ A_p + A_p \circ dF^{-1} + dF \circ B_p \circ dF \ ,$$

$$P_p^+ = \frac{1}{2} (D_\varphi + i dF) \circ \Theta_p \circ (\Theta_p + i dF) \ ,$$

$$\frac{1}{2} (J_p \circ \partial F - i \partial F) = (\Theta_p + i dF) \circ B_p \circ (\Theta_p + i dF) \ ,$$

where

$$\Theta_p = B_p^{-1} \circ (D_\varphi - i A_p) = C \circ (D_\varphi - i A)^{-1} \ ,$$

$$\Theta_p^T = \Theta_p \ , \ \Theta_p \circ D_\pi = D_\pi \circ \Theta_p = 0 \ .$$

Using Eq. (2.97), we find conditions for positive resp. negative frequency solutions in the language of quantities on $\Sigma$ only:

$$(\Theta_p + idF) \circ \phi^- = 0 \ , \ (\Theta_p^* - idF) \circ \phi^+_p = 0 \ .$$

We see that the value and normal derivative on $\Sigma$ of positive resp. negative frequency solutions are “proportional” to each other through the bi-form $\Theta_p$ which is uniquely given by $J_p$ and the choice of the hypersurface $\Sigma$. It means that the value of the field on a hypersurface $\Sigma$ is enough to determine the positive resp. negative frequency solution.

Remembering properties (2.51) and (2.45), (2.46) we can formulate conditions for $G_p^+$

$$(\Theta_p + idF) \circ G_p^+ = 0 \ , \ G_p^+ \circ (\Theta_p + idF) = 0 \ ,$$

$$(\Theta_p + idF) \circ G_p^- = 0 \ , \ G_p^- \circ (\Theta_p^* - idF) = 0 \ .$$
Here it does not matter on which hypersurface we formulate boundary conditions. Using relations (2.48) we get a set of conditions which uniquely determine the Feynman Green function

\[-i (\chi[\Omega]\delta) \bullet F \bullet \mathcal{G}^F_p = (\chi[\Omega]\delta),\]

\[(\Theta_p[\Sigma_f^+ - idF[\Sigma_f]] \bullet \mathcal{G}^F_p \bullet (\chi[\Omega]\delta) = 0),\]

\[(\chi[\Omega]\delta) \bullet \mathcal{G}^F_p \bullet (\Theta_p[\Sigma_i] + idF[\Sigma_i]) = 0,\]

(2.102)

for any domain \(\Omega = \langle \Sigma_f|\Sigma_i \rangle\) and we recovered explicit dependence on hypersurfaces which is important for boundary conditions for the Feynman Green function.

### 3 In-out formalism

**Two particle interpretations**

Until now we have investigated a single particle interpretation of the scalar field theory. But there exist a lot of different particle interpretations, each corresponding to a different complex structure on the phase space, and in a general situation none of them have a preferred position.

However in most physical situations, we are dealing with spacetime which has special properties at least in the remote past and future. For example, the spacetime may be static in these regions. It gives us the possibility to choose a preferred notion of particles in the past and in the future. These particle interpretations are not generally the same. It is usual to call one of these notions of particles “in” (or initial) particles and other one “out” (or final) particles. We have to face a natural physical question of what is the relation of these two kinds of particles.

Therefore we need to investigate a relation of two particle interpretation. This problem is usually described in terms of Bogoljubov coefficients. We will reformulate the theory using quantities independent on a choice of a bases of modes, and we will also find connections among different in-out Green functions and their geometrical interpretation similar to the interpretation of Green functions associated with the one-particle interpretation. We will also find that given a Green function with certain properties, we are able to reconstruct two particle interpretations for which the Green function is an in-out Green function.

**Green functions**

Let us choose two particle interpretations given by two complex structures \(J_i\) and \(J_f\). We will change the letter “\(p\)” to the letters “\(i\)” resp. “\(f\)” in all quantities defined in the part 2. It means that we have two, generally different, vacuum states \(|i : vac\rangle, |f : vac\rangle\), two sets of creation and annihilation operators etc.

We can define new Green functions, beside \(G^{(1)}_i, G^+_i, G^F_i, G^{(1)}_f, G^+_f, G^F_f\). Let’s define in-out Hadamard Green function

\[G^{(1)}_{xy} = \frac{\langle f : vac|\hat{\Phi}^x\hat{\Phi}^y + \hat{\Phi}^y\hat{\Phi}^x|i : vac\rangle}{\langle f : vac|i : vac\rangle},\]  
(3.1)

Wightman functions

\[G^{+xy} = \frac{\langle f : vac|\hat{\Phi}^x\hat{\Phi}^y|i : vac\rangle}{\langle f : vac|i : vac\rangle}, \quad G^{-xy} = \frac{\langle f : vac|\hat{\Phi}^y\hat{\Phi}^x|i : vac\rangle}{\langle f : vac|i : vac\rangle}\]  
(3.2)
and Feynman Green function

\[ G^F_{xy} = \frac{\langle f : vac | T (\hat{\Phi}^x \hat{\Phi}^y) | i : vac \rangle}{\langle f : vac | i : vac \rangle}. \]  \hspace{1cm} (3.3)

Similar relations to Eqs. (2.43-2.49) hold among these Green functions except relations (2.46), i.e.

\[ G^{(1)} = G^+ + G^- , \quad G_C = i(G^+ - G^-) , \]  \hspace{1cm} (3.4)

\[ G^+ = \frac{1}{2}(G^{(1)} - iG_C) , \quad G^- = \frac{1}{2}(G^{(1)} + iG_C) , \]  \hspace{1cm} (3.5)

\[ G^{+ T} = G^- , \quad G^{(1) T} = G^{(1)} , \quad G^{F T} = G^F , \quad G_C^T = -G_C , \]  \hspace{1cm} (3.6)

\[ G^F = -i\bar{G} + \frac{1}{2}G^{(1)} , \]  \hspace{1cm} (3.7)

\[ G^F_{xy} = \begin{cases} G^+_{xy} & \text{for } x \text{ after } y , \\ G^-_{xy} & \text{for } x \text{ before } y , \\ G^{+xy} = G^{-xy} = \frac{1}{2}G^{(1)xy} & \text{for } x, y \text{ space-like separated} \end{cases} . \]  \hspace{1cm} (3.8)

\[ F \bullet G^{(1)} = 0 , \quad F \bullet G^\pm = 0 , \]
\[ -i(\chi[\Omega]\delta) \bullet F \bullet G^F = (\chi[\Omega]\delta) . \]  \hspace{1cm} (3.9)

Let us define operators \( J \) and \( P^\pm \) on \( \Gamma^C \) using equations similar to Eqs. (2.54), (2.55)

\[ P^\pm = \mp iG^\pm \circ \partial F , \]
\[ J = G^{(1)} \circ \partial F = i(P^+ - P^-) . \]  \hspace{1cm} (3.10)

Using the fact that a positive frequency part of \( \hat{\Phi} \) annihilates a vacuum we get

\[ G^+ = P^+_F \circ G^+ = G^+ \circ P^-_i , \quad G^- = P^-_i \circ G^- = G^- \circ P^+_f , \]  \hspace{1cm} (3.12)

therefore

\[ P^+ = P^+_F \circ P^+ = P^+ \circ P^+_i , \quad 0 = P^-_i \circ P^+ = P^+ \circ P^-_i , \]
\[ P^- = P^-_i \circ P^- = P^- \circ P^-_f , \quad 0 = P^+_i \circ P^- = P^- \circ P^+_f . \]  \hspace{1cm} (3.13)

and finally

\[ P^\pm \circ P^\mp = 0 , \quad G^\pm \circ \partial F \circ G^\mp = 0 . \]  \hspace{1cm} (3.14)

From Eq. (3.4) we get

\[ P^+ + P^- = \delta \]  \hspace{1cm} (3.15)

and it, together with previous equation, gives

\[ P^\pm \circ P^\pm = P^\pm , \quad G^\pm \circ \partial F \circ G^\pm = \pm iG^\pm , \]  \hspace{1cm} (3.16)
\[ J \circ J = -\delta , \quad G^{(1)} \circ \partial F \circ G^{(1)} = G_C . \]  \hspace{1cm} (3.17)

We can further show

\[ P^\pm \circ \partial F \circ P^\pm = 0 , \quad J \circ \partial F = -\partial F \circ J . \]  \hspace{1cm} (3.18)
We see that $J$ is a complex structure compatible with $\partial F$, and $P^\pm$ are its eigenspace projectors. However, there is a difference from the complex structures $J_i$ or $J_f$ — the complex structure $J$ does not act on the space $\Gamma$ but on the complexified space $\Gamma^C$. More precisely, in general $J^* \neq J$, $G^{(1)*} \neq G^{(1)}$, $P^\pm \neq P^\mp$, $G^{\pm*} \neq G^\mp$. Therefore the complex structure $J$ does not define a particle interpretation (except, of course, in the degenerate case $J_f = J_i = J$).

We can define real and imaginary parts of the complex structure $J$

$$J = M + iN \quad ,$$

$$M = \text{Re} J = \frac{1}{2}(J + J^*) \quad , \quad N = \text{Im} J = -i\frac{1}{2}(J - J^*) \quad ,$$

Using Eqs. (3.15), (3.13) and their complex conjugates and previous definitions we get

$$M = i(P^+ - P^-) = i(P^-* - P^-) \quad ,$$

$$N = P^+ + P^-* - \delta = \delta - P^- - P^-*$$

and

$$-J_f \circ M = -M \circ J_i = \delta + N \quad , \quad -M \circ J_f = -J_i \circ M = \delta - N \quad .$$

This gives us an important relation

$$[-\frac{1}{2}(J_i + J_f)] \circ M = M \circ [-\frac{1}{2}(J_i + J_f)] = \delta \quad ,$$

or

$$\frac{1}{2}(G^{(1)} + G^{(1)*}) = [\frac{1}{2}(\gamma_i + \gamma_f)]^{-1} = -G_C \circ [\frac{1}{2}(G_i^{(1)} + G_f^{(1)})]^{-1} \circ G_C \quad .$$

We will define a real symmetric bi-form $\gamma$

$$\gamma = [\text{Re} G^{(1)}]^{-1} = \frac{1}{2}(\gamma_i + \gamma_f) \quad .$$

This means that $\gamma$, and therefore also $\text{Re} G^{(1)}$, are positive definite. We define a real scalar product on the phase space $\Gamma$ and a corresponding transposition using the bi-form $\gamma$

$$(\phi_1, \phi_2) = \phi_1^T \circ \phi_2 = \phi_1 \circ \gamma \circ \phi_2 \quad \text{for} \quad \phi_1, \phi_2 \in \Gamma \quad ,$$

$$A^T = \gamma^{-1} \circ A \circ \gamma \quad \text{for} \quad A \in \Gamma_1^1 \quad .$$

From Eqs. (3.17), (3.18) follow

$$M \circ \partial F = -\partial F \circ M \quad , \quad N \circ \partial F = -\partial F \circ N \quad ,$$

$$-\delta = M \circ M - N \circ N + i(M \circ N + N \circ M)$$

i.e.

$$N \circ N = \delta + M \circ M \quad ,$$

$$M \circ N = -N \circ M \quad .$$

Now it is straightforward to show that $N$ is symmetric and $M$ is antisymmetric with respect of the transposition (3.26). If we define the absolute value $|M|$ and signum $\sigma$ of the operator $M$

$$|M| = (M^T \circ M)^{\frac{1}{2}} = (-M \circ M)^{\frac{1}{2}} \quad ,$$

$$\sigma = \text{sign} M = M \circ |M|^{-1} = |M|^{-1} \circ M \quad ,$$

19
we find

\[ \sigma^T = \sigma^{-1} \quad , \quad \sigma^* = \sigma \quad , \quad |M|^T = |M| \quad , \quad |M|^* = |M| \quad , \]

(3.33)

\[ \sigma \circ \partial F = - \partial F \circ \sigma \quad , \quad |M| \circ \partial F = \partial F \circ |M| \quad , \]

(3.34)

\[ \sigma \circ \sigma = - \delta \quad , \quad \sigma \circ \partial F \quad \text{is positive definite} \quad , \]

(3.35)

\[ [ |M|, N] = 0 \quad , \quad \sigma \circ N = - N \circ \sigma \quad , \quad \sigma \circ |M| = |M| \circ \sigma \quad . \]

(3.36)

Therefore $|M|$ and $N$ have common eigenvectors and can be written as functions of a single operator. We can find this operator solving Eq. (3.29).

The Green function can be written in the form (3.1), where the initial and final complex structures are given by (3.42).

This is true also in an opposite direction. Any Green function which satisfies these conditions is possible to write in the form (3.1), where the initial and final complex structures are given by (3.42).

We will see below that the operator $X$ is closely connected with Bogoljubov transformation. Finally we can express initial and final complex structures

\[ J_i = \exp(-X) \circ \sigma = \sigma \circ \exp(X) \quad , \quad J_f = \exp(X) \circ \sigma = \sigma \circ \exp(-X) \quad , \]

(3.42)

and using this we see that $X$ is $i$-antilinear, $f$-antilinear and symmetric:

\[ X \circ J_i = - J_i \circ X \quad , \quad X \circ J_f = - J_f \circ X \quad , \quad X^{(T)} = X \quad . \]

(3.43)

We have found that the Hadamard Green function $G^{(1)}$ defined by Eq. (3.1) satisfies

\[ F \bullet G^{(1)} = 0 \quad , \quad G^{(1)T} = G^{(1)} \quad , \]

(3.44)

\[ G^{(1)} \circ \partial F \circ G^{(1)} = G_C \quad , \]

(3.45)

\[ \gamma = [\text{Re} G^{(1)}]^{-1} \quad \text{is positive definite} \quad . \]

(3.46)

This is true also in an opposite direction. Any Green function which satisfies these conditions is possible to write in the form (3.1), where the initial and final complex structures are given by (3.42).

We can also find boundary conditions for in-out Feynman Green function similarly to Eq. (2.102). Using Eqs. (3.8), (3.12) and (2.103) we get

\[ -i (\chi[\Omega] \delta) \bullet F \bullet G^F = (\chi[\Omega] \delta) \quad , \]

(3.47)

\[ (\Theta_f[\Sigma_f]^* - i \hat{F}[\Sigma_f]) \bullet G^F \bullet (\chi[\Omega] \delta) = 0 \quad , \]

\[ (\chi[\Omega] \delta) \bullet G^F \bullet (\Theta_f[\Sigma_f]^* - i \hat{F}[\Sigma_f]) = 0 \quad , \]

\[ (\Theta_i[\Sigma_i] + i \hat{F}[\Sigma_i]) \bullet G^F \bullet (\chi[\Omega] \delta) = 0 \quad , \]

\[ (\chi[\Omega] \delta) \bullet G^F \bullet (\Theta_i[\Sigma_i] + i \hat{F}[\Sigma_i]) = 0 \quad . \]

for any domain $\Omega = (\Sigma_f/\Sigma_i)$.

The relations among projectors $P^\pm_i, P^\pm_f, P^\pm_j$ and the operator $J$ can be translated to composition laws among Green function. Beside Eqs. (3.16), (3.17) we have, for example (using Eq. (3.13))

\[ G^+_f \circ \partial F \circ G^+ = \pm i G^+ \quad , \quad G^+ \circ \partial F \circ G^+_i = \mp i G^+ \quad . \]

(3.48)
Bogoljubov operators

We have studied the relation of two particle interpretations from the point of view of Green functions. Now we will compare initial and final creation and annihilation operators.

Because the structures of initial and final particle interpretations are generated by creation and annihilation operators which satisfy the same commutation relations, we can expect that they are related by a unitary transformation. In other words, for any experiment formulated using the initial notion of particles, we can construct an experiment formulated in the same way using the final notion of particles. These experiments will be generally different, but their description should be related by a unitary transformation.

However this “translation” of the initial experiment to the final one is not unique. We have to specify which initial and final states correspond each other. We have to specify, for example, how we change modes which we use for labeling of one-particle states.

More precisely, we write a relation of initial and final particle states in following way

$$|f : \text{vac}\rangle = \hat{S}^\dagger |i : \text{vac}\rangle,$$  \hspace{1cm} (3.49)

$$\hat{a}_f [s \circ \phi]^\dagger |f : \text{vac}\rangle = \hat{S}^\dagger \hat{a}_i [\phi]^\dagger |i : \text{vac}\rangle,$$  \hspace{1cm} (3.50)

where $\hat{S}$ is a unitary operator on the quantum space $\mathcal{H}$ called the S-matrix,

$$\hat{S}^\dagger = \hat{S}^{-1},$$  \hspace{1cm} (3.51)

and $s$ is a transition operator on the phase space $\Gamma$ which “translates” initial modes to final modes as we discussed above. This means that an initial one-particle state labeled by a mode $\phi$ is related by a unitary transformation given by the S-matrix with a final one-particle state labeled by the mode $s \circ \phi$. Of course, the S-matrix depends on a choice of the operator $s$.

The relation (3.49), (3.50) are equivalent to

$$\hat{a}_f [s \circ \phi]^\dagger = \hat{S}^\dagger \hat{a}_i [\phi]^\dagger \hat{S},$$  \hspace{1cm} (3.52)

Using the commutation relation (2.10) and unitarity of the S-matrix we get a condition on the operator $s$,

$$\langle s \circ \phi_1, s \circ \phi_2 \rangle_f = \langle \phi_1, \phi_2 \rangle_i.$$  \hspace{1cm} (3.53)

The operator $s$ changes the initial scalar product on the phase space $\Gamma$ to the final one. This is a natural condition which expresses a meaning of the transition operator $s$ — this operator translates the initial labeling of one-particle states to the final one, and therefore it has to map all initial structures on the phase space to the final ones. Consequences of the last equation are

$$s \circ \gamma_f \circ s = \gamma_i, \quad s \circ \partial F \circ s = \partial F, \quad J_f \circ s = s \circ J_i.$$  \hspace{1cm} (3.54)

Using these relations and Eq. (3.52) we can get another relation between the S-matrix and the operator $s$,

$$s \circ \hat{\Phi} = \hat{S} \hat{\Phi} \hat{S}^\dagger.$$  \hspace{1cm} (3.55)

The transition operator $s$ is closely related to Bogoljubov coefficients between initial and final bases of modes. It can be seen from a decomposition of $s$ to $i$-linear and $i$-antilinear parts (see Eqs. (2.24), (2.25))

$$s = \alpha + \beta,$$  \hspace{1cm} (3.56)

$$\alpha \circ J_i = J_i \circ \alpha, \quad \beta \circ J_i = -J_i \circ \beta.$$  \hspace{1cm} (3.57)

Explicitly

$$\alpha = \frac{1}{2} (s - J_i \circ s \circ J_i) = P_i^+ \circ s \circ P_i^+ + P_i^- \circ s \circ P_i^-,$$  \hspace{1cm} (3.58)

$$\beta = \frac{1}{2} (s + J_i \circ s \circ J_i) = P_i^+ \circ s \circ P_i^- + P_i^- \circ s \circ P_i^+.$$
This allows us to write relations of initial and final positive and negative frequency projectors,
\[ P_i^+ \circ s = P_i^+ \circ \alpha + P_i^- \circ \beta, \]
\[ P_i^- \circ s = P_i^- \circ \alpha + P_i^+ \circ \beta, \]  \hspace{1cm} (3.59)
and relations of initial and final creation and annihilation operators,
\[ \hat{a}_f[s \circ \phi] = \hat{a}_i[\alpha \circ \phi] - \hat{a}_i[\beta \circ \phi], \]
\[ \hat{a}_f[s \circ \phi]^\dagger = \hat{a}_i[\alpha \circ \phi]^\dagger - \hat{a}_i[\beta \circ \phi]. \]  \hspace{1cm} (3.60)

This expresses final creation resp. annihilation operators as a mixture of both initial creation and annihilation operators. It shows explicitly that the initial and final notion of particles are really different for \( \beta \neq 0 \).

We will call this choice of \( \alpha, \beta \) **Bogoljubov operators**.

Now we will investigate properties of Bogoljubov operators. It is straightforward to show (see Eqs. (2.26), (2.27) and (2.28) for definition of used operations)
\[ s^{-1} = -J_i \circ s^T_i \circ J_i = \alpha^{(T)}_i - \beta^{(T)}_i, \]
\[ s \circ s^{T_i} = -J_f \circ J_i. \]  \hspace{1cm} (3.61), (3.62)
Substituting this and Eq. (3.56) to \( \delta = s \circ s^{-1} = s^{-1} \circ s \) and taking \( i \)-linear and \( i \)-antilinear parts we get identities
\[ \alpha \circ \alpha^{(I)}_i - \beta \circ \beta^{(T)}_i = \delta, \]
\[ \alpha^{(I)}_i \circ \alpha - \beta^{(T)}_i \circ \beta = \delta. \]  \hspace{1cm} (3.63), (3.64)

The transition operator \( s \) is not fixed by Eq. (3.53) uniquely, we have a freedom in selecting this operator. It corresponds to a freedom in labeling of our one-particle states. We can change the labeling of initial one-particle states by \( i \)-unitary transformation of the phase space without changing the initial notion of particles and similarly with the final particles. If we have two different transition operators \( s_a \) and \( s_b \) for translation of initial modes to final modes, they both have to satisfy Eq. (3.53) and we easily see that they have to be related by
\[ s_a = s_b \circ u_i = u_f \circ s_b, \]  \hspace{1cm} (3.65)
where \( u_i \) resp. \( u_f \) is an \( i \)-linear and \( i \)-antilinear resp. \( f \)-linear and \( f \)-unitarian operator on the phase space \( \Gamma \) (see Eqs. (2.24), (2.26)).

All equations can be simplified if we choose a special transition operator \( s \). The operator
\[ s_o = \exp(\mathcal{X}) = -\sigma \circ J_i = -J_f \circ \sigma = [-J_f \circ J_i]^{\frac{1}{2}} \]  \hspace{1cm} (3.66)
satisfies conditions (3.54) and therefore also the condition (3.53), and so we can use it as a special transition operator for translation of initial to final modes. We will call this choice canonical. We can define canonical Bogoljubov operators \( \alpha_o, \beta_o \) by Eq. (3.58) and using Eq. (3.54), we get
\[ s_o = \exp(\mathcal{X}) = \alpha_o + \beta_o, \]
\[ s_o^{-1} = \exp(-\mathcal{X}) = \alpha_o - \beta_o, \]  \hspace{1cm} (3.67)
\[ \alpha_o = \cosh \mathcal{X}, \quad \beta_o = \sinh \mathcal{X}, \]  \hspace{1cm} (3.68)
\[ \alpha_o \circ J_i = J_i \circ \alpha_o, \quad \beta_o \circ J_i = -J_i \circ \beta_o, \]  \hspace{1cm} (3.69)
\[ s_o^{T_i} = s_o, \quad \alpha_o^{(T)} = \alpha_o, \quad \beta_o^{(T)} = \beta_o. \]  \hspace{1cm} (3.70)

We also see that the operators \( \alpha_o \) and \( -\beta_o \) play a role of inverse canonical Bogoljubov operators for transformation from final to initial particle states.
This is possible to generalize for any transition operator $s$. Using Eq. (3.65) we get

$$s = \exp(\mathcal{X}) \circ u_i = u_f \circ \exp(\mathcal{X}) = \alpha + \beta,$$

$$s^{-1} = \exp(-\mathcal{X}) \circ u_i = u_f \circ \exp(-\mathcal{X}) = \alpha^{(t)} - \beta^{(T)},$$

$$\alpha \circ J_{i,f} = J_{i,f} \circ \alpha,$$

$$\beta \circ J_{i,f} = -J_{i,f} \circ \beta. \quad (3.72)$$

We see that the inverse Bogoljubov operators are $\alpha^{(t)}$ and $-\beta^{(T)}$. Finally, let us note that

$$\beta \circ \alpha^{-1} = \alpha^{-1} \circ \beta = \tanh \mathcal{X} = N. \quad (3.73)$$

Now we will show a connection with standard Bogoljubov coefficients. Let’s assume that a $i$-orthonormal resp $f$-orthonormal bases $u = \{u_k; k \in \mathcal{I}\}$ resp. $v = \{v_k; k \in \mathcal{I}\}$ for description of initial resp. final modes are chosen. It defines the transition operator $s$ by the conditions

$$v_k = s \circ u_k, \quad J_f \circ v_k = s \circ J_i \circ u_k \quad (3.74)$$

for all $k \in \mathcal{I}$. The Bogoljubov coefficients $\alpha_{kl}, \beta_{kl}$ are defined by the equations

$$v_k^+ = \sum_{k \in \mathcal{I}} (u_i^+ \alpha_{lk} + u_i^- \beta_{lk}). \quad (3.75)$$

Using Eq. (3.59) we see

$$\alpha_{kl} = \langle u_k, \alpha \circ u_i \rangle_i, \quad \beta_{kl} = \langle u_k, \beta \circ u_i \rangle_i,$$

i.e. Bogoljubov coefficients are matrix elements of the Bogoljubov operators in a chosen base.

We can use eigenvectors of the operator $\mathcal{X}$ to define special bases of initial and final modes — so called canonical bases [10]. Because the operator $\mathcal{X}$ is $i$-symmetric it has a complete set of eigenvectors. From $i$-antilinearity follows that for each eigenvector $u$ the vector $J_i \circ u$ is also an eigenvector with the opposite sign of the eigenvalue. Therefore we can choose an $\mathbb{R}$-base $\{u_k, J_i \circ u_k; k \in \mathcal{I}\}$ such that

$$\mathcal{X} \circ u_k = \chi_k u_k, \quad \chi_k \geq 0,$$

$$\mathcal{X} \circ J_i \circ u_k = -\chi_k J_i \circ u_k. \quad (3.77)$$

The base can be chosen orthonormal with respect to the real scalar product defined by the bi-form $\gamma_i$

$$u_k \circ \gamma_i \circ u_l = \delta_{kl}, \quad u_k \circ \gamma_i \circ J_i \circ u_l = 0. \quad (3.78)$$

If the operator $\mathcal{X}$ is nondegenerate with different eigenvalues, the base is fixed uniquely. The subset $\{u_k; k \in \mathcal{I}\}$ of this $\mathbb{R}$-base forms the $i$-orthonormal $\mathbb{C}$-base. It will be used for labeling of initial particles. The final $f$-orthonormal $\mathbb{C}$-base $\{v_k; k \in \mathcal{I}\}$ will be generated by the canonical transition operator $s_o$, 

$$v_k = s_o \circ u_k = \exp(\chi_k) u_k. \quad (3.79)$$

The Bogoljubov transformation between these two bases is

$$v_k^+ = u_k^+ \cosh(\chi_k) + u_k^- \sinh(\chi_k) \quad (3.80)$$

and the final and initial creation and annihilation operators are related by

$$\hat{a}_f[v_k] = \hat{a}_i[u_k] \cosh(\chi_k) - \hat{a}_i[u_k]^\dagger \sinh(\chi_k),$$

$$\hat{a}_f^*[v_k] = \hat{a}_i[u_k]^\dagger \cosh(\chi_k) - \hat{a}_i[u_k] \sinh(\chi_k). \quad (3.81)$$
Transition amplitudes

Now we are prepared to calculate in-out transition amplitudes, i.e. amplitudes between initial and final particle states. It is possible to show (see [1, 3]) that amplitudes between many particle states can be reduced to one particle transition amplitudes. Therefore we will calculate only these simple amplitudes.

First, using Eq. (3.60) and its inversion, we get identities

\begin{align}
\hat{a}_i[\phi]^\dagger &= \hat{a}_f[s \circ \alpha^{-1} \circ \phi]^\dagger + \hat{a}_i[\beta \circ \alpha^{-1} \circ \phi] \\
\hat{a}_f[\phi] &= \hat{a}_i[s^{-1} \circ \alpha^{-1}(t) \circ \phi] - \hat{a}_f[\beta^T \circ \alpha^{-1}(t) \circ \phi]^\dagger.
\end{align}

(3.82)

Now it is easy to check that vacuum – one-particle transition amplitudes vanish

\begin{align}
\langle f : vac|\hat{a}_i[\phi]^\dagger|i : vac \rangle &= \langle f : vac|\hat{a}_f[s \circ \alpha^{-1} \circ \phi]^\dagger + \hat{a}_i[\beta \circ \alpha^{-1} \circ \phi]|i : vac \rangle = 0 \\
\langle f : vac|\hat{a}_f[\phi]|i : vac \rangle &= 0.
\end{align}

(3.83)

The one-particle to one-particle transition amplitude is

\begin{align}
\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]^\dagger|i : vac \rangle &= \frac{\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]^\dagger|i : vac \rangle}{\langle f : vac|i : vac \rangle} \\
&= \frac{\langle f : vac|\hat{a}_i[s \circ \phi_1]^{\dagger}\hat{a}_f[s \circ \alpha^{-1} \circ \phi_2] + \hat{a}_i[\beta \circ \alpha^{-1} \circ \phi_2]|i : vac \rangle}{\langle f : vac|i : vac \rangle} = \langle s \circ \phi_1, s \circ \alpha^{-1} \circ \phi_2 | i = \phi_1 \circ \Lambda \circ \phi_2 \\
\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]|i : vac \rangle &= -\langle \phi_1, \alpha^{-1} \circ \beta \circ \phi_2 | i = \phi_1 \circ V \circ \phi_2.
\end{align}

(3.84)

where we have used the commutation relation (2.10). Vacuum to two-particle transition amplitudes are

\begin{align}
\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]^\dagger|i : vac \rangle &= \frac{\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]^\dagger|i : vac \rangle}{\langle f : vac|i : vac \rangle} \\
&= \frac{\langle f : vac|\hat{a}_i[s \circ \phi_1]^{\dagger}\hat{a}_f[s \circ \alpha^{-1} \circ \phi_2] + \hat{a}_i[\beta \circ \alpha^{-1} \circ \phi_2]|i : vac \rangle}{\langle f : vac|i : vac \rangle} = \langle \beta \circ \alpha^{-1} \circ \phi_1, \phi_2 | i = \phi_1 \circ \Lambda \circ \phi_2 \\
\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]|i : vac \rangle &= -\langle \phi_1, \alpha^{-1} \circ \beta \circ \phi_2 | i = \phi_1 \circ V \circ \phi_2.
\end{align}

(3.85)

We have introduced amplitudes I, V, \Lambda similarly to De Witt’s notation [3]

\begin{align}
I &= -i P_i^- \circ \partial F \circ \alpha^{-1} \circ P_i^+ \\
\Lambda &= i P_i^+ \circ \partial F \circ \tanh(X) \circ P_i^- \\
V &= i P_i^- \circ \partial F \circ \tanh(X) \circ P_i^+.
\end{align}

(3.87)

The bi-form V, and \Lambda are independent of a choice of the operator s, and I is s-dependent.

These expressions are connected more closely with initial modes — we have used a transition operator s to generate final modes. It is possible to also obtain translation amplitudes without this asymmetry. Simply choosing the canonical operator s_0 and doing some algebra, we can get

\begin{align}
\langle f : vac|\hat{a}_f[s \circ \phi_1]\hat{a}_i[\phi_2]^\dagger|i : vac \rangle &= \langle \delta - \tanh X \circ \phi_1, \phi_2 | i = \langle \phi_1, (\delta + \tanh X) \circ \phi_2 | f = \\
&= -\langle \phi_1 \circ \partial F \circ G^+ \circ \partial F \circ \phi_2.
\end{align}

(3.88)
\[
\langle f : \text{vac} | \hat{a}_i^\dagger \hat{a}_i | i : \text{vac} \rangle = \langle \text{tanh}(x) \circ \phi_1, \phi_2 \rangle_i = \frac{1}{2} \phi_1 \circ P_i^+ \circ \partial F \circ G^{(1)} \circ \partial F \circ P_i^+ \circ \phi_2 ,
\]
\[
\langle f : \text{vac} | i : \text{vac} \rangle = \frac{1}{2} \phi_1 \circ P_i^+ \circ \partial F \circ G^{(1)} \circ \partial F \circ P_i^+ \circ \phi_2 .
\]

We have thus calculated the in-out one-particle transition amplitudes, except for calculating the normalization factor \( \langle f : \text{vac} | i : \text{vac} \rangle \). In [1] (see also [3]) it is derived that
\[
\langle f : \text{vac} | i : \text{vac} \rangle = (\det \Gamma \cosh x)^{-\frac{1}{2}} = (\det \Gamma_{i,f} \cosh x)^{-\frac{1}{2}} = \left( \prod_{k \in I} \cosh \chi_k \right)^{-\frac{1}{2}} .
\] (3.91)

Other interesting physical quantities are the mean number of final particles in the initial vacuum. Using the identities (3.60) we get
\[
\langle i : \text{vac} | \hat{n}_f[s \circ \phi] | i : \text{vac} \rangle = \frac{\langle \beta \circ \phi, \beta \circ \phi \rangle_i}{\langle \phi, \phi \rangle_i} = \frac{\langle \sinh(x) \circ \phi, \sinh(x) \circ \phi \rangle_i}{\langle \phi, \phi \rangle_i}.
\] (3.92)
or
\[
\langle i : \text{vac} | \hat{n}_f[\phi] | i : \text{vac} \rangle = \frac{\langle \sinh(x) \circ \phi, \sinh(x) \circ \phi \rangle_f}{\langle \phi, \phi \rangle_f} .
\] (3.93)

and similarly
\[
\langle f : \text{vac} | \hat{n}_i[\phi] | f : \text{vac} \rangle = \frac{\langle \sinh(x) \circ \phi, \sinh(x) \circ \phi \rangle_i}{\langle \phi, \phi \rangle_i} .
\] (3.94)

The mean total number of particles is
\[
\langle i : \text{vac} | \hat{N}_f | i : \text{vac} \rangle = \sum_{k \in I} \langle i : \text{vac} | \hat{n}_f[v_k] | i : \text{vac} \rangle = \sum_{k \in I} \langle v_k, (\sinh x)^2 \circ v_k \rangle_f
\] (3.95)
for some \( f \)-orthonormal \( \mathbb{C} \)-base, i.e.
\[
\langle i : \text{vac} | \hat{N}_f | i : \text{vac} \rangle = \text{Tr}_{f^*} (\sinh x)^2 = \sum_{k \in I} (\sinh \chi_k)^2
\] (3.96)
and similarly
\[
\langle f : \text{vac} | \hat{N}_i | f : \text{vac} \rangle = \text{Tr}_{f^*} (\sinh x)^2 = \sum_{k \in I} (\sinh \chi_k)^2 .
\] (3.97)

The regularity of this quantity guarantees the unitary equivalence of the initial and final particle representations of the quantum algebra and regularity of the vacuum – vacuum amplitude (3.91) (see [3, 11]).
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Notes

1 We will denote \( \mathfrak{F} M \) the space of the functions on manifold \( M \), \( \tilde{\mathfrak{F}}^\alpha M \) the space of densities on \( M \) of a weight \( \alpha \). If \( V \) is a vector space and \( V^* \) its dual, \( V^k \) will denote the tensor space

\[
\frac{V \otimes \cdots \otimes V \otimes V^* \otimes \cdots \otimes V^*}{k \text{ times}}.
\]

2 \( \phi \) means an abstract vector from \( \mathfrak{H} \) with coordinates \( \Phi(x) = \phi(x) \). The coordinates of a covector \( \omega(x) \) are densities on the manifold \( M \).

3 We are using MTW \[15\] signs conventions and geometric units \( c = 1, \) \( \hbar = 1 \). Greek indexes \((\alpha, \beta, \gamma, \ldots)\) are used for spacetime tensors, latin letters from the beginning of alphabet \((a, b, c, \ldots)\) for space tensors and from the end of alphabet \((\ldots, x, y, z)\) for spacetime points. In rare occasions when we will need indexes for vectors from \( \Gamma \) we will use also letters \( \ldots, x, y, z \). Bold indexes represent abstract vector indexes in the sense of Penrose \[16\]. Plain indexes are coordinate indexes.

4 The delta distribution \( \delta(x-x') = \delta(x|x') \) is a density in one point and function in other one, \( (\delta(x-x') \phi x) \) is a density in both points and \( (\chi[\Omega] \delta \psi) \) is a projection on the domain \( \Omega \) (i.e. \( (\chi[\Omega] \delta \psi = \chi[\Omega] \psi) \)). The distributions \( \delta \phi, \delta \omega \) are distributions representing gradients of delta function defined by

\[
\varphi^\alpha \cdot \delta \phi^\alpha = \int \varphi^\alpha \omega(x) dx,
\]

\[
\varphi^\alpha \cdot \delta \omega^\alpha = \int \varphi^\alpha \phi(x) dx.
\]

for any test function \( \psi \in \mathfrak{F} M \) and test vector density \( \varphi^\alpha \). Similarly \( \Box \) is the d’Alembert operator acting on delta function.

5 We are using following convention for operators \((A \in \Gamma_1^1, \phi \in \Gamma, \omega \in \Gamma_0^1)\)

\[
\omega \circ A \circ \phi = \omega(x) A^y_y \phi^y ,
\]

\[
\phi \circ A \circ \omega = \phi^y A^x_y \omega(x) .
\]

It means that in the first case the operator \( A \) acts to the right, in the later case to the left. The order is determined by the fact that \( \phi \) is vector and \( \omega \) is covector. This convention simulate contraction of vector indexes and it is necessary to be careful in some cases. For example if \( A, B \) are operators on \( \Gamma \) we can write

\[
(A \circ \partial F \circ GC \circ B)^y_x = A^u_y \partial F_u z G_{xy} B^u_x = -A^u_y \delta^{(u)}_u B^v_x = -(B \circ A)^y_x \neq -(A \circ B)^y_x .
\]

6 Here the “gradient” \( \delta \) acts on the phase space \( \Gamma \).

7 Because for the description of a scalar field we need bosonic particles, we are assuming only the bosonic version of Fock space.
8 More precisely we should use here the symbol $\delta^{(\Gamma)}$ for the identity operator on $\Gamma$ as we did before. We will omit a superscript if it is clear from context that we are speaking about operators on $\Gamma$.

9 We cannot write simply

$$-iF \bullet G_p^F = \delta$$

(similarly for $G_{ret}, G_{adv}$ and $G$) because for $\phi \in \Gamma$ we would get

$$\phi = \phi \bullet \delta = \phi \bullet (-i)F \bullet G_p^F = 0$$

using the equation of motion (1.2). $F$ has zero eigenvectors (exactly the phase space $\Gamma$) and therefore it does not have an inverse tensor.

We could use Eq. (*) if we understood $F_{xz} G^F_{zy}$ as a distribution in the argument $x$ acting only on test functions with compact support. The step function $\chi[\Omega]$ supply this conditions even for $\phi \in \Gamma$ which does not have a compact support, but it produces new important boundary terms and therefore the improved equation (2.50) does not lead to the contradiction (**).

$$\phi \bullet (\chi[\Omega] \delta) = -i \phi \bullet (\chi[\Omega] \delta) \bullet F \bullet G_p^F =$$

$$=-i \phi \bullet F \bullet (\chi[\Omega] \delta) \bullet G_p^F - i \phi \bullet \partial F[\partial \Omega] \bullet G_p^F =$$

$$=-i \phi \bullet \partial F[\Sigma_J] \bullet G^+ \bullet (\chi[\Omega] \delta) + i \phi \bullet \partial F[\Sigma_I] \bullet G^- \bullet (\chi[\Omega] \delta) =$$

$$= \phi \bullet \partial F[\Sigma] \bullet G_C \bullet (\chi[\Omega] \delta) = \phi \bullet (\chi[\Omega] \delta)$$

where we have used equations (2.50), (1.3), (2.48), (2.43) and (1.10).

10 Polar decomposition is a decomposition of an operator in a Hilbert space into its absolute value and signum. We will use it for a real Hilbert space, i.e. a real vector space with a scalar product defined by a symmetric positive quadratic form $h$

$$(a,b) = a^T \cdot b = a \cdot h \cdot b \quad a,b \text{ vectors} \; , \; \quad A^T = h^{-1} \cdot A \cdot h \quad A \text{ an operator} \; .$$

There exists unique left resp. right decomposition of an operator $O$

$$O = |O|_l \cdot \operatorname{sign}_l O = \operatorname{sign}_r O \cdot |O|_r$$

to a positive definite symmetric operator $|O|_l$ resp. $|O|_r$ and an orthogonal operator $\operatorname{sign}_l O$ resp. $\operatorname{sign}_r O$

$$|O|_{l,r}^{T} = |O|_{l,r} \; , \; \quad |O|_{l,r} \text{ positive definite} \; , \; \quad (\operatorname{sign}_{l,r} O)^T = (\operatorname{sign}_{l,r} O)^{-1}$$

and these operators are given by

$$|O|_l = (O \cdot O^T)^{\frac{1}{2}} \; , \; \quad |O|_r = (O^T \cdot O)^{\frac{1}{2}} \; , \; \quad \operatorname{sign}_l O = |O|^{-1}_l \cdot O \; , \; \quad \operatorname{sign}_r O = O \cdot |O|^{-1}_r$$

If $O$ commutes with $O^T$ both decompositions coincide.
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