On the Relation Between Fock and Schrödinger Representations for a Scalar Field

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Linear free field theories are one of the few Quantum Field Theories that are exactly soluble. There are, however, (at least) two very different languages to describe them, Fock space methods and the Schrödinger functional description. In this paper, the precise sense in which the two representations are related is reviewed. Several properties of these representations are studied, among them the well known fact that the Schrödinger counterpart of the usual Fock representation is described by a Gaussian measure. A real scalar field theory is considered, both on Minkowski spacetime for arbitrary, non-inertial embeddings of the Cauchy surface, and for arbitrary (globally hyperbolic) curved spacetimes. As a concrete example, the Schrödinger representation on stationary and homogeneous cosmological spacetimes is constructed.

PACS numbers: 03.70.+k, 04.62.+v

I. INTRODUCTION

In ordinary quantum theory, a state is represented by a vector $|\Psi\rangle$ in an abstract Hilbert space $\mathcal{H}$, and observables are represented by Hermitian operators on $\mathcal{H}$. For a finite dimensional system –such as a harmonic oscillator– with a configuration space with coordinates $q^i$, there are at least two equivalent representations of the Hilbert space. One can represent the quantum states as wave functions $\psi(q^i) = \langle q^i|\Psi\rangle$ of the configuration space, in what is known as the Schrödinger picture; alternatively, one can consider the basis $|\vec{n}\rangle$ such that a state is given by $\langle \vec{n}|\Psi\rangle$, where the kets $|\vec{n}\rangle$ are eigen-kets of the Hamiltonian: $\hat{H}|\vec{n}\rangle = E(\vec{n})|\vec{n}\rangle$. In this case, the state is characterized by the countable array of numbers $\langle \vec{n}|\Psi\rangle$. Given the basis $|\vec{n}\rangle$, and a general state $|\Psi\rangle = \sum_{\vec{n}} A_{\vec{n}}|\vec{n}\rangle$ one can then write $\langle q^i|\Psi\rangle = \sum_{\vec{n}} A_{\vec{n}}\langle q^i|\vec{n}\rangle$. Using the relation $\langle q^i|\Psi\rangle = \sum_{\vec{n}} (\langle q^i|\vec{n}\rangle \langle \vec{n}|\Psi\rangle)$, we conclude that $A_{\vec{n}} = \langle \vec{n}|\Psi\rangle$. When we have knowledge of the eigenfunctions as in the case of a harmonic oscillator where $\langle q^i|\vec{n}\rangle = H_{\vec{n}}(q^i)$, we have a natural passage from the ‘Fock’ representation $\langle \vec{n}|\Psi\rangle$ to the Schrödinger wavefunction $\langle q^i|\Psi\rangle$. In this case both representations are well defined and understood. A natural generalization of these two descriptions for mechanical systems is to go to field theory. In this case, the situation becomes more involved, due to the existence of an infinite number of degrees of freedom. In the ordinary presentation of field theory, it is the Fock representation the one that is more intuitive and widely known, whereas the Schrödinger is not equally treated. This paper has as its main motivation the desire of presenting, in a clear fashion, both representations for a scalar field theory and their relation.

The reason to study the quantum theory of a free real scalar field is that it is one of the simplest field theory systems. Indeed, it is studied in the first chapters on most field theory textbooks. The language used for these treatments normally involves Fourier decomposition of the field and creation and annihilation operators associated with an infinite chain of harmonic oscillators. Canonical quantization is normally performed by representing these operators on Fock space and implementing the Hamiltonian operator. On the other hand, books that introduce QFT from an axiomatic viewpoint, normally deal either with functional Euclidean methods or with abstract algebras and states in the algebraic approach. All these approaches deal with QFT on a flat Minkowski spacetime. An intermediate treatment, motivated by the the process of quantization, starting from a classical algebra of observables and constructing representations of them on Hilbert spaces, studies quantum fields on curved spacetimes. This
approach, closely related to the classical “canonical quantization” methods of Dirac, is somewhat complementary to the standard viewpoint. In the mentioned book, Wald develops the quantum theory of a scalar field, and extends the formalism to an arbitrary curved manifold. His construction is, however, restricted to finding a representation on Fock space, or as is normally known, the Fock representation.

On the other side of the program of canonical quantization for fields, is the Schrödinger representation, where a slicing of the spacetime is normally introduced (for reviews see [8]). This functional viewpoint, even when popular in the past, is not widely used, in particular since it is not the most convenient one for performing calculations of physical scattering processes in ordinary QFT. However, from the conceptual viewpoint, the study of the Schrödinger representation in field theory is extremely important and has not been, from our viewpoint widely acknowledged (however, see [9]). This is specially true since some symmetry reduced gravitational systems can be rewritten as the theory of a scalar field on a fiducial, flat, background manifold. In particular, of recent interest are the polarized Einstein-Rosen waves [10] and Gowdy cosmologies [11]. In this regard, the Schrödinger picture is, in a sense, the most natural representation from the viewpoint of canonical quantum gravity, where one starts from the outset with a decomposition of spacetime into a spatial manifold Σ “evolving in time”. Therefore, it is extremely important to have a good understanding of the mathematical constructs behind this representation and its relation to the Fock representation.

The purpose of this paper is twofold. The first one is to review and present the relation between the Fock and Schrödinger representations of a scalar field on Minkowski spacetime, in a coherent and unified manner. We recall basic constructions at both the classical and quantum levels, and develop from a logical viewpoint the precise sense in which the representations are related. In particular, we show in detail the way in which the quantum measure in the functional picture arises and its Gaussian character. In the process, we emphasize the relevant geometrical objects that need to be specified in order to define both representations and its relation. In this regard, the present work can be considered as a review. The emphasis in our presentation regarding this extra structure allows us to achieve the second purpose of the paper, namely, to extend the formalism to arbitrary embeddings of the Cauchy surface and to arbitrary curved spacetimes, in the spirit of [6]. The generalization is at two levels. To be specific, both the existing ambiguity in the quantization of a scalar field, and the infinite freedom in the choice of embedding of the Cauchy surface are considered. We construct the relation between these two representations and give concrete examples for background spacetimes that are of physical interest. These later results are, to the best of our knowledge, rather new and not widely available.

The structure of the paper is as follows. In Sec. II we recall basic notions from canonical quantization and the classical formulation of a scalar field. In Sec. III we recall the ordinary Fock representation in the spirit of [6]. A discussion of the Schrödinger representation and construction of the theory unitary equivalent to a given Fock representation is the subject of Section IV. In Sec. V we show the relation between the two equivalent representations in an explicit fashion. In Sec. VI we present several examples of spacetimes for which the Schrödinger representation is explicitly constructed. We end with a discussion in Sec. VII. In a series of appendixes, we prove some of the results presented in the main text.

In order to make this work accessible not only to specialized researchers in theoretical physics, we have intentionally avoided going into details regarding functional analytic issues and other mathematically sophisticated constructions. Instead, we refer to the specialized literature and use those results in a less sophisticated way, emphasizing at each step their physical significance. This allows us to present our results in a self-contained fashion.

Throughout the paper we shall use units such that $G = c = 1$ and the abstract index notation for tensorial objects.

II. PRELIMINARIES

In this section we shall present some background material, both in classical and quantum mechanics. This section has two parts. In the first one we recall some basic notions of symplectic geometry that play a fundamental role in the Hamiltonian description of classical systems, and outline the canonical quantization starting from a classical system. In the second part, we recall the phase space description for a scalar field.

1 However, it has been successfully used for proving a variety of results that do not need dynamical information.
A. Canonical Quantization

A physical system is normally represented, at the classical level, by a phase space, consisting of a manifold $\Gamma$ of even dimension. The symplectic two-form $\Omega$ endows it with the structure of a symplectic space $(\Gamma, \Omega)$. The symplectic structure $\Omega$ defines the Poisson bracket $\{\cdot, \cdot\}$ on the observables, that is, on functions $f, g : \Gamma \to \mathbb{R}$, in the usual way:

$$\{f, g\} = \Omega^{ab}\nabla_a f \nabla_b g.$$  

In very broad terms, by quantization one means the passage from a classical system, to a quantum system. Observables on $\Gamma$ are to be promoted to self-adjoint operators on a Hilbert space. However, we know that not all observables can be promoted unambiguously to quantum operators satisfying the Canonical Commutation Relations (CCR). A well known example of such problem is factor ordering. What we can do is to construct a subset $\mathcal{S}$ of elementary classical variables for which the quantization process has no ambiguity. This set $\mathcal{S}$ should satisfy two properties:

- $\mathcal{S}$ should be a vector space large enough so that every (regular) function on $\Gamma$ can be obtained by (possibly a limit of) sums of products of elements in $\mathcal{S}$. The purpose of this condition is that we want that enough observables are to be unambiguously quantized.
- The set $\mathcal{S}$ should be small enough such that it is closed under Poisson brackets.

The next step is to construct an (abstract) quantum algebra $\mathcal{A}$ of observables from the vector space $\mathcal{S}$ as the free associative algebra generated by $\mathcal{S}$ (for a definition and discussion of free associative algebras see [13]). It is in this quantum algebra $\mathcal{A}$ that we impose the Dirac quantization condition: Given $A, B$ and $\{A, B\}$ in $\mathcal{S}$ we impose,

$$[\hat{A}, \hat{B}] = i\hbar \{A, B\}. \quad (2.1)$$

It is important to note that there is no factor order ambiguity in the Dirac condition since $A, B$ and $\{A, B\}$ are contained in $\mathcal{S}$ and they have associated a unique element of $\mathcal{A}$.

The last step is to find a Hilbert space $\mathcal{H}$ and a representation of the elements of $\mathcal{A}$ as operators on $\mathcal{H}$. For details of this approach to quantization see [14].

In the case that the phase space $\Gamma$ is a linear space, there is a particular simple choice for the set $\mathcal{S}$. We can take a global chart on $\Gamma$ and we can choose $\mathcal{S}$ to be the vector space generated by linear functions on $\Gamma$. In some sense this is the smallest choice of $\mathcal{S}$ one can take. As a concrete case, let us look at the example of $\mathbb{R}^3$. We can take a global chart on $\Gamma$ given by $(q^i, p_i)$ and consider $\mathcal{S} = \text{Span}\{1, q^1, q^2, q^3, p_1, p_2, p_3\}$. It is a seven dimensional vector space. Notice that we have included the constant functions on $\Gamma$, generated by the unit function since we know that $\{q^i, p_i\} = 1$, and we want $\mathcal{S}$ to be closed under Poisson brackets (PB).

We can now look at linear functions on $\Gamma$. Denote by $Y^a$ an element of $\Gamma$, and using the fact that it is linear space, $Y^a$ also represents a vector in $TT$. Given a one form $\lambda_a$, we can define a linear function on $\Gamma$ as follows: $F_{\lambda}(Y) := -\lambda_a Y^a$. Note that $\lambda$ is a label of the function with $Y^a$ as its argument. First, note that there is a vector associated to $\lambda_a$:

$$\lambda^a := \Omega^{ab}\lambda_b,$$

so we can write

$$F_{\lambda}(Y) = \Omega_{ab}\lambda^a Y^b = \Omega(\lambda, Y). \quad (2.2)$$

If we are now given another label $\nu$, such that $G_{\nu}(Y) = -\nu_a Y^a$, we can compute the PB

$$\{F_{\lambda}, G_{\nu}\} = \Omega_{ab}\nabla_a F_{\lambda}(Y) \nabla_b G_{\nu}(Y) \Omega^{ab}\lambda_a \nu_b. \quad (2.3)$$

Since the two-form is non-degenerate we can rewrite it as $\{F_{\lambda}, G_{\nu}\} = -\Omega_{ab}\lambda^a \nu^b$. Thus,

$$\{\Omega(\lambda, Y), \Omega(\nu, Y)\} = -\Omega(\lambda, \nu). \quad (2.4)$$

As we shall see in Sec. [113] we can also make such a selection of linear functions for the Klein-Gordon field.

The quantum representation is the ordinary Schrödinger representation where the Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3, d^3x)$ and the operators are represented by:

$$\langle \hat{1} \cdot \Psi \rangle(q) = \Psi(q) \quad \langle \hat{q}^i \cdot \Psi \rangle(q) = q^i \Psi(q) \quad \langle \hat{p}_i \cdot \Psi \rangle(q) = -i\hbar \frac{\partial}{\partial q^i} \Psi(q). \quad (2.5)$$

Thus, we recover the conventional quantum theory in the Schrödinger representation.
B. Phase Space and Observables for a scalar field

In this part we shall recall the phase space and Hamiltonian description of a real, linear Klein-Gordon field $\phi(x^\mu)$. In this paper we shall assume that we are in Minkowski spacetime, so the theory we are considering is defined on $^4M$. We will perform a $3+1$ decomposition of the spacetime in the form $M = \Sigma \times R$, for $\Sigma$ any Cauchy surface, which in this case is topologically $R^3$. We will consider arbitrary embeddings of the surfaces $\Sigma$ into $^4M$. The first step is to write the classical action for the field,

$$S := -\frac{1}{2} \int_M (g^{ab} \nabla_a \phi \nabla_b \phi + m^2 \phi^2) \sqrt{|g|} \, d^4x.$$ \hspace{1cm} (2.6)

The field equation is then,

$$\langle \nabla^a \nabla_a - m^2 \rangle \phi = 0.$$ \hspace{1cm} (2.7)

Next, we decompose the spacetime metric as follows: $g^{ab} = h^{ab} - n^a h^b$. Here $h^{ab}$ is the (inverse of) the induced metric on the Cauchy hypersurface $\Sigma$ and $n^a$ the unit normal to $\Sigma$. We also introduce an everywhere time-like vector field $t^a$ and a ‘time’ function $t$ such that the hypersurfaces $t = \text{constant}$ are diffeomorphic to $\Sigma$ and such that $t^a \nabla_a t = 1$.

Note that, for each $t$, we have an embedding of the form $T_t : \Sigma \rightarrow ^4M$. Thus, a choice of function $t$ provides a one-parameter family of embeddings (a foliation of $^4M$). We can write $t^a = N n^a + a^a$. The volume element is given by $\sqrt{|g|} \, d^4x = N \sqrt{h} \, d^3x$. Using these identities in Eq. (2.6) we get,

$$S = \frac{1}{2} \int_I \int_\Sigma N \sqrt{h} \left[ (n^a \nabla_a \phi)^2 - h^{ab} \nabla_a \phi \nabla_b \phi - m^2 \phi^2 \right] \, d^3x,$$ \hspace{1cm} (2.8)

where $I = [t_0, t_1]$ is an interval in the real line. Using the relation

$$n^a \nabla_a \phi = \frac{1}{N} (t^a - N^a) \nabla_a \phi = \frac{1}{N} \dot{\phi} - \frac{1}{N} N^a \nabla_a \phi,$$

we can conclude then that the momentum density $\pi$, canonically conjugate to the configuration variable $\phi$ on $\Sigma$, is given by

$$\pi = \frac{\delta S}{\delta \phi} \sqrt{h} (n^a \nabla_a \phi).$$ \hspace{1cm} (2.9)

The phase space $\Gamma$ of the theory can thus be written as $\Gamma = (\varphi, \pi)$, where the configuration variable $\varphi$ is the restriction of $\phi$ to $\Sigma$ and $\pi$ is $\sqrt{h} n^a \nabla_a \phi$ restricted to $\Sigma$. Note that the phase space is of the form $\Gamma = T^* C$, where the classical configuration space $C$ can be taken as suitable initial data (for instance, smooth functions of compact support).

There is an alternative description for the phase space of the theory, given by the “covariant phase space” \[15\]. In this approach, the phase space is the space of solutions $\phi$ to the equation of motion. Let us denote this space by $\Gamma_s$. Note that, for each embedding $T_t : \Sigma \rightarrow ^4M$, there exists an isomorphism $T_t$ between $\Gamma$ and $\Gamma_s$. The key observation is that there is a one to one correspondence between a pair of initial data of compact support on $\Sigma$, and solutions to the Klein-Gordon equation on $^4M$ \[15\].

Therefore, to each element $\phi$ in $\Gamma_s$ there is a pair $(\varphi, \pi)$ on $\Gamma$ ($\varphi = T^*_t [\phi]$ and $\pi = T^*_t \left[ \sqrt{h} n^a \nabla_a \phi \right]$) and conversely, for each pair, there is a solution to the Klein-Gordon equation that induces the given initial data on $\Sigma$.

In the phase space $\Gamma$ the symplectic structure $\Omega$ takes the following form, when acting on vectors $(\varphi_1, \pi_1)$ and $(\varphi_2, \pi_2)$,

$$\Omega(\varphi_1, \pi_1, \varphi_2, \pi_2) = \int_\Sigma (\pi_1 \varphi_2 - \pi_2 \varphi_1) \, d^3x.$$ \hspace{1cm} (2.10)

Observables for the space $\Gamma$ can be constructed directly by giving smearing functions on $\Sigma$. We can define linear functions on $\Gamma$ as follows: given a vector $Y^\alpha$ in $\Gamma$ of the form $Y^\alpha = (\varphi, \pi)^\alpha$, and a pair $\lambda_\alpha = (-f, -g)_\alpha$, where $f$ is a scalar density and $g$ a scalar, we define the action of $\lambda$ on $Y$ as,

$$F_\lambda(Y) = -\lambda_\alpha Y^\alpha := \int_\Sigma (f \varphi + g \pi) \, d^3x.$$ \hspace{1cm} (2.11)

Now, we can write this linear function in the form $F_\lambda(Y) = \Omega_{\alpha \beta} \lambda^\alpha Y^\beta = \Omega(\lambda, Y)$, if we identify $\lambda^\beta = \Omega^{\beta \alpha} \lambda_\alpha = (-g, f)^\beta$. That is, the smearing functions $f$ and $g$ that appear in the definition of the observables $F$ and are therefore
naturally viewed as a 1-form on phase space, can also be seen as the vector \((-g, f)\). Note that the role of the smearing functions is interchanged in the passing from a 1-form to a vector. Of particular importance for what follows is to consider configuration and momentum observables. They are particular cases of the observables \(F\) depending of specific choices for the label \(\lambda\). Let us consider the “label vector” \(\lambda^\alpha = (0, f)^\alpha\), which would be normally regarded as a vector in the “momentum” direction. However, when we consider the linear observable that this vector generates, we get,

\[
\varphi[f] := \int_{\Sigma} d^2 x f \varphi.
\] (2.12)

Similarly, given the vector \((-g, 0)^\alpha\) we can construct,

\[
\pi[g] := \int_{\Sigma} d^2 x g \pi.
\] (2.13)

Note that any pair of test fields \((-g, f)^\alpha \in \Gamma\) defines a linear observable, but they are ‘mixed’. More precisely, a scalar \(g\) in \(\Sigma\), that is, a pair \((-g, 0) \in \Gamma\) gives rise to a momentum observable \(\pi[g]\) and, conversely, a scalar density \(f\), which gives rise to a vector \((0, f) \in \Gamma\) defines a configuration observable \(\varphi[f]\). In order to avoid possible confusions, we shall make the distinction between label vectors \((-g, f)^\alpha\) and coordinate vectors \((\varphi, \pi)^\alpha\).

As we have seen, the phase space can be alternatively described by solutions to the Klein-Gordon equation in the covariant formalism (\(\Gamma_s\)) or by pairs of fields on a Cauchy surface \(\Sigma\) in the canonical approach (\(\Gamma\)). In both cases, the elements of the algebra \(\mathcal{S}\) to be quantized are linear functionals of the basic fields. In the following sections we consider the construction of the quantum theory, both in the Fock and in the Schrödinger representation.

### III. FOCK QUANTIZATION

Let us now consider the Fock quantization. The intuitive idea is that the Hilbert space of the theory is constructed from “n-particle states”. (In certain cases one is justified to interpret the quantum states as consisting of n-particle states.) The Fock quantization is naturally constructed from solutions to the classical equations of motion and relies heavily on the linear structure of the space of solutions (The Klein-Gordon equation is linear). Thus, it can only be implemented for quantizing linear (free) field theories. In the following sections we consider the construction of the quantum theory, both in the Fock and in the Schrödinger representation.

The classical observables to be quantized are the fundamental fields which correspond to exact solutions of Eq.(2.7). The next step in the quantization program is to identify the one-par ticle Hilbert space \(\mathcal{H}_0\) from the space \(\Gamma_s\), as we will see below the only input that we require to construct \(\mathcal{H}_0\) is to introduce a complex structure compatible with the naturally defined symplectic structure on \(\Gamma_s\). As mentioned before, the one-particle Hilbert space \(\mathcal{H}_0\) receives this name since it can be interpreted as the Hilbert space of a one-particle relativistic system. From the Hilbert space \(\mathcal{H}_0\) one constructs its symmetric (since we are considering Bose fields) Fock space \(\mathcal{F}_s(\mathcal{H}_0)\), the Hilbert space of the theory. The final step is to represent the quantum version of the algebra \(\mathcal{S}\) of observables in the Fock space as suitable combinations of (naturally defined) creation and annihilation operators.

The classical observables to be quantized are the fundamental fields \(\Phi\) which correspond to exact solutions of Eq.(2.7). The next step in the quantization program is to identify the one-particle Hilbert space \(\mathcal{H}_0\). The strategy is the following: start with \((\Gamma_s, \Omega)\) a symplectic vector space and define \(J : \Gamma_s \rightarrow \Gamma_s\), a linear operator such that \(J^2 = -1\). The complex structure \(J\) has to be compatible with the symplectic structure. This means that the bilinear mapping defined by \(\mu(\cdot, \cdot) := \Omega(J\cdot, \cdot)\) is a positive definite metric on \(\Gamma_s\). The Hermitian (complex) inner product is then given by,

\[
\langle \cdot, \cdot \rangle = \frac{1}{2\hbar}\mu(\cdot, \cdot) - i\frac{1}{2\hbar}\Omega(\cdot, \cdot).
\] (3.1)

The complex structure \(J\) defines a natural splitting of \(\Gamma_s\), the complexification of \(\Gamma_s\), in the following way: Define the positive frequency part to consist of vectors of the form \(\Phi^+ := \frac{1}{2}(\Phi - iJ\Phi)\), and the negative frequency part as \(\Phi^- := \frac{1}{2}(\Phi + iJ\Phi)\). Note that \(\Phi^- = \overline{\Phi}^+\) and \(\Phi = \Phi^+ + \Phi^-\). Since \(J^2 = -1\), the eigenvalues of \(J\) are \(\pm i\), so one is decomposing the vector space \(\Gamma_s\) in eigenspaces of \(J\): \(J(\Phi^\pm) = \pm \Phi^\mp\). We have used the term ‘positive-negative frequency’ since in the case of the Minkowski spacetime the naturally defined \(J\) induces this standard decomposition (See Sec. VI).

There are two alternative but completely equivalent descriptions of the one-particle Hilbert space \(\mathcal{H}_0\):
\( \mathcal{H}_0 \) consists of real valued functions (solution to the Klein-Gordon equation for instance), equipped with the complex structure \( J \). The inner product is given by \( \langle \Phi, \Phi \rangle = -\frac{i}{\hbar} \Omega(\Phi^-, \Phi^+) \).

\( \mathcal{H}_0 \) is constructed by complexifying the vector space \( \Gamma_n \) (tensoring with the complex numbers) and then decomposing it using \( J \) as described above. In this construction, the inner product is given by,

\[
\langle \Phi, \check{\Phi} \rangle = -\frac{i}{\hbar} \Omega(\Phi^-, \check{\Phi}^+) .
\]

Note that in this case, the one-particle Hilbert space consists of ‘positive frequency’ solutions.

It is important to note that the only input we needed in order to construct \( \mathcal{H}_0 \) was the complex structure \( J \).

The symmetric Fock space associated to \( \mathcal{H}_0 \) is defined to be the Hilbert space

\[
\mathcal{F}_s(\mathcal{H}_0) := \bigoplus_{n=0}^{\infty} \left( \bigotimes_n \mathcal{H}_0 \right) ,
\]

where we define the symmetrized tensor product of \( \mathcal{H}_0 \), denoted by \( \bigotimes^n \mathcal{H}_0 \), to be the subspace of the n-fold tensor product \( (\bigotimes^n \mathcal{H}_0) \), consisting of totally symmetric maps \( \alpha : \overline{\mathcal{H}}_1 \times \cdots \times \overline{\mathcal{H}}_n \rightarrow C \) (with \( \mathcal{H}_1 = \cdots = \mathcal{H}_n = \mathcal{H}_0 =: \mathcal{H} \)) satisfying

\[
\sum |\alpha(\bar{e}_{i_1}, \ldots, \bar{e}_{i_n})|^2 < \infty .
\]

The Hilbert space \( \overline{\mathcal{H}} \) is the complex conjugate of \( \mathcal{H} \) with \( \{\bar{e}_1, \cdots, \bar{e}_j, \cdots\} \) an orthonormal basis. We are also defining \( \bigotimes^0 \mathcal{H} = C \).

We shall introduce the abstract index notation for the Hilbert spaces since it is the most convenient way of describing the Fock space. Given a space \( \mathcal{H} \), we can construct the spaces \( \overline{\mathcal{H}} \), the complex conjugate space; \( \mathcal{H}^* \), the dual space; and \( \overline{\mathcal{H}}^* \) the dual to the complex conjugate. In analogy with the notation used in spinors, let us denote elements of \( \mathcal{H} \) by \( \phi^A \), elements of \( \overline{\mathcal{H}} \) by \( \phi^{A'} \). Similarly, elements of \( \mathcal{H}^* \) are denoted by \( \phi_A \) and elements of \( \overline{\mathcal{H}}^* \) by \( \phi_A' \). However, by using Riesz lemma, we may identify \( \overline{\mathcal{H}} \) with \( \mathcal{H}^* \) and \( \mathcal{H} \) with \( \overline{\mathcal{H}}^* \). Therefore we can eliminate the use of primed indices, so \( \phi_A \) will be used for an element in \( \overline{\mathcal{H}}^* \) corresponding to the element \( \phi^A \in \mathcal{H} \). An element \( \phi \in \bigotimes^n \mathcal{H} \) then consists of elements satisfying

\[
\phi^{A_1 \cdots A_n} = \phi^{(A_1 \cdots A_n)} .
\]

An element \( \psi \in \bigotimes^n \overline{\mathcal{H}} \) will be denoted as \( \psi_{A_1 \cdots A_n} \). In particular, the inner product of vectors \( \psi, \phi \in \mathcal{H} \) is denoted by

\[
\langle \psi, \phi \rangle := \overline{\psi}_A \phi^A .
\]

A vector \( \Psi \in \mathcal{F}_s(\mathcal{H}) \) can be represented, in the abstract index notation as

\[
\Psi = (\psi, \psi^{A_1}, \psi^{A_1 A_2}, \ldots, \psi^{A_1 \cdots A_n}, \ldots) ,
\]

where, for all \( n \), we have \( \psi^{A_1 \cdots A_n} = \psi^{(A_1 \cdots A_n)} \). The norm is given by

\[
|\Psi|^2 := \overline{\psi}_A \psi^A + \overline{\psi}_{A_1 A_2} \psi^{A_1 A_2} + \cdots < \infty .
\]

Now, let \( \xi^A \in \mathcal{H} \) and let \( \xi_A \) denote the corresponding element in \( \overline{\mathcal{H}} \). The annihilation operator \( \mathcal{A}(\xi) : \mathcal{F}_s(\mathcal{H}) \rightarrow \mathcal{F}_s(\mathcal{H}) \) associated with \( \xi_A \) is defined by

\[
\mathcal{A}(\xi) \cdot \Psi := (\xi_A \psi^A, \sqrt{2} \xi_A \psi^{A A_1}, \sqrt{3} \xi_A \psi^{A A_1 A_2}, \ldots) .
\]

Similarly, the creation operator \( \mathcal{C}(\xi) : \mathcal{F}_s(\mathcal{H}) \rightarrow \mathcal{F}_s(\mathcal{H}) \) associated with \( \xi^A \) is defined by

\[
\mathcal{C}(\xi) \cdot \Psi := (0, \psi^{A_1}, \sqrt{2} \xi^{(A_1; A_2)}, \sqrt{3} \xi^{(A_1; A_2 A_3)}, \ldots) .
\]

If the domains of the operators are defined to be the subspaces of \( \mathcal{F}_s(\mathcal{H}) \) such that the norms of the right sides of Eqs. (3.4) and (3.5) are finite then it can be proven that \( \mathcal{C}(\xi) = (\mathcal{A}(\xi^A))^\dagger \). It may also be verified that they satisfy the commutation relations,

\[
[\mathcal{A}(\xi), \mathcal{C}(\eta)] = \xi_A \eta^A \mathbf{1} .
\]
A more detailed treatment of Fock spaces can be found in [6, 12, 16, 17].

In the previous section we saw that we could construct linear observables in \((\Gamma, \Omega)\), which we denoted by \(F_\lambda(Y)\). These observables are given by \(\mathcal{O}[\eta]\) and in the more canonical picture by \(\mathcal{A} = \mathcal{A}[\eta]\) and \(\mathcal{C}[\eta]\). This is the set \(\mathcal{S}\) of observables, now denoted by \(\mathcal{O}[\eta]\), for which there will correspond a quantum operator. Thus, for \(\mathcal{O}[\eta] \in \mathcal{S}\) there is an operator \(\hat{\mathcal{O}}[\eta]\). We want the CCR to hold, 

\[
\left[\hat{\mathcal{O}}[\eta], \hat{\mathcal{O}}[\xi]\right] = i\hbar (\mathcal{O}[\eta], \mathcal{O}[\xi]) \hat{1} - i\hbar \Omega(\eta, \xi) \hat{1}.
\]  

(3.7)

Then we should see that the Fock construction is a Hilbert space representation of our basic operators satisfying the above conditions. We have all the structure needed at our disposal. Let us take as the Hilbert space the symmetric Fock space \(\mathcal{F}_s(H)\) and let the operators be represented as

\[
\hat{\mathcal{O}}[\eta] \cdot \Psi := i\hbar (\mathcal{A}(\eta) - \mathcal{C}(\eta)) \cdot \Psi.
\]  

(3.8)

Let us denote by \(\eta^A\) the abstract index representation corresponding to the pair \((-g, f)\) in \(H\). That is, the vector \(\eta\) appearing in the previous expressions should be thought of as a label for the state created (or annihilated) by \(\mathcal{C}(\eta)\) or \(\mathcal{A}(\eta)\) on the Hilbert space.

Let us now focus on the properties of the operators given by \(\mathcal{A}\). First, note that by construction the operator is one to one correspondence between them, and that \(J\) represents the (infinite) freedom in the choice of the quantum representation.

IV. SCHRÖDINGER REPRESENTATION

In the previous section we considered the Fock quantization of the Klein-Gordon field, one of its most notable features being the fact that it is most naturally stated and constructed in a covariant framework. In particular, the symplectic structure, even when it uses explicitly a hypersurface \(\Sigma\), is independent of this choice. The same is true for the complex structure which is a mapping from solutions to solutions. The infinite dimensional freedom in choice of representation of the CCR relies in the choice of admissible \(J\), which gives rise to the one-particle Hilbert space. Thereafter, the construction is completely natural and there are no further choices to be made. We know that from the infinite possible choices of \(J\) there are physically inequivalent representations \([18]\), a clear indication that the Stone-von Neumann theorem does not generalize to field theories.

We now turn our attention to the Schrödinger representation. In contrast to the previous case, this construct relies heavily on a Cauchy surface \(\Sigma\), since its most naive interpretation is in terms of a “wave functional at time \(t\).” For simplicity, we have assumed that we are in Minkowski spacetime, so the theory we are considering is defined on \(\Sigma \times R\). However, we are considering arbitrary embeddings, so the surface \(\Sigma\) is topologically \(R^3\), but can have an arbitrary metric \(h_{ab}\), and extrinsic curvature on it. Recall that the phase space of the theory can be written as \(\Gamma = (\varphi, \pi)\), where \(\varphi = T^*_\pi \phi\) and \(\pi = T^*_\varphi \sqrt{\det g} \nabla_c \phi\). Recall that in this case the phase space is of the form \(\Gamma = T^*C\), where the classical configuration space \(C\) can be taken as suitable initial data (for instance, smooth functions of compact support). The results reported in this section follow \([18]\) closely.

A. First Steps

The Schrödinger representation, at least in an intuitive level, is to consider ‘wave functions’ as function(al)s of \(\varphi\). That is

\[
\mathcal{H}_s := L^2(C, d\mu),
\]  

(4.1)
where a state would be represented by a function(al) \( \Psi[\varphi]: \mathcal{C} \to \mathbb{C} \).

We have already encountered two new actors in the play. First comes the quantum configuration space \( \mathcal{C} \), and the second one is the measure \( \mu \) thereon. Thus, one will need to specify these objects in the construction of the theory. Before going into that, let us look at the classical observables that are to be quantized, and in terms of which the CCR are expressed. Recall the observables \( \varphi[f]\) and \( \pi[g] \),

\[
\varphi[f] := \int_\Sigma d^3x \; f \varphi
\]

and

\[
\pi[g] := \int_\Sigma d^3x \; g \pi,
\]

where the test functions \( g \) and \( f \) are again smooth and of compact support. The Poisson bracket between the configuration and momentum observables is,

\[
\{\varphi[f], \pi[g]\} = \int d^3x \; f g,
\]

so the canonical commutation relations read \( [\hat{\varphi}[f], \hat{\pi}[g]] = i\hbar \int d^3x \; f g \hat{I} \).

Recall that in the general quantization procedure the next step is to represent the abstract operators \( \hat{\varphi}[f] \) and \( \hat{\pi}[g] \) as operators in a Hilbert space, with the appropriate “reality conditions”, which in our case means that these operators should be Hermitian.

We can represent them, when acting on functionals \( \Psi[\varphi] \) as

\[
(\hat{\varphi}[f] \cdot \Psi)[\varphi] := \varphi[f] \Psi[\varphi],
\]

and

\[
(\hat{\pi}[g] \cdot \Psi)[\varphi] := -i\hbar \int d^3x \; g(x) \frac{\delta \Psi}{\delta \varphi(x)} + \text{multiplicative term}.
\]

The second term in (4.4), depending only on configuration variable is there to render the operator self-adjoint when the measure is different from the “homogeneous” measure, and depends on the details of the measure. At this point we must leave it unspecified since we have not defined the measure yet.

In quantum mechanics, we are used to the fact that we can simply take the same measure (Lebesgue) on \( R^3 \) for an ordinary problem and not even worry about this issue. We are saved in that case by the Stone-von Neumann theorem that assures us that any ‘decent’ representation of the CCR is unitarily equivalent to the Schrödinger one. In field theory this is false. There are infinitely inequivalent representations of the CCR. In the Fock representation we saw that the ambiguity is encoded in the complex structure \( J \). However, in the Schrödinger picture we encounter the first conceptual difficulty. How does the infinite ambiguity existent manifest itself in the Schrödinger picture? Intuitively, one expects that the information be somehow encoded in the measure \( \mu \), which will, by the reality conditions, manifest itself in the choice of the representation of the momentum operator \( \hat{J} \). This intuitive picture gets entangled however with two features that were absent in the Fock construction. The first one is that one is tempted to apply an old trick which is very useful in, say, a harmonic oscillator in QM. Recall that in that case, one can either consider the Hilbert space \( L^2(R, dq) \) of square integrable functions with respect to the Lebesgue measure \( dq \), in which case one has the representation of the operators as in (4.5). The vacuum is given by a Gaussian of the form \( \psi_0(q) = \exp(-q^2/2) \). The other possibility is to “incorporate the vacuum” into the measure, in such a way that the measure becomes now \( dq' = \exp(-q^2) dq \), and the vacuum is the unit function \( \psi_0(q) = 1 \). With this choice, the momentum operator acquires an extra term such that \( \hat{p} = -i\hbar(d/dq - i\frac{1}{2} \hat{q}) \). The two representations are completely equivalent since one can go from any wave-function \( \psi(q) \) in the standard representation to a state in the new representation by \( \psi \mapsto \psi(q) = \exp(q^2/2) \psi \).

This map is a unitary isomorphism of Hilbert spaces and thus the two representations are equivalent. The question now is whether one can apply such a map in the functional case, and go from a ‘simple’ representation with uniform measure to a ‘complicated’ representation with a non-uniform measure, in a unitary way. (See [13] for the construction of the vacuum state for the case of the Klein-Gordon field.)

The second feature that was briefly mentioned before has to do with the fact that one is defining the theory on a particular Cauchy surface and therefore there might be extra complications coming from a non-standard choices of embeddings. That is, in the covariant picture the complex structure is independent of any such hypersurface, and might induce very different looking maps, in terms of initial data, for different choices of \( \Sigma \). In what follows we shall
see that one can overcome these difficulties and define a canonical representation of the CCR, in terms of what is normally referred to as the associated Gaussian measure.

In order to understand the situation, let us explore what appears to be the simplest and most attractive possibility, namely let us consider the case in which the measure is the uniform one. That is, the measure can be written something like \(d\mu = D\varphi\), and would be the equivalent of the Lebesgue measure in the real line. In this case, the momentum operator is represented as follows:

\[
\hat{p}[g] = -i\hbar \int d^3x \, g(x) \frac{\delta}{\delta \varphi(x)}.
\]

From our experience with the harmonic oscillator, we expect that the vacuum be a Gaussian wave function (see B). If we regard the quantization as a recipe for producing a Hilbert space and a representation of the basic operators, we are finished! There is however something very puzzling about this construct. It appears to be universal for any scalar field theory over \(\Sigma\); there is no trace of the ambiguity present in the Fock picture, namely of the complex structure \(J\). Have we somehow been able to get something as a “free lunch”, and been able to circumvent the difficulty? The answer is in the negative and there are at least two aspects to it. Heuristically, we can see that we have not been completely successful in the construction, since we have failed to provide the vacuum state \(\Psi_0(\varphi)\). This suggests that the information about the \(J\), and therefore, the different possible “representations” is encoded in the choice of vacuum and not in the representation itself. If this were the case, then inequivalence of the different representations would manifest itself as the impossibility to define a unitary map connecting the different vacuum states. This explanation seems plausible and, as we shall see later, has some concrete use. In fact this is the standard issue of “choice of the vacuum” that one finds in standard texts [7]. However, there is still a deeper reason why this naive representation is ‘wrong’. From a technical point of view, this representation with a “uniform” measure is not well defined for the simple reason that such measure does not exist!

The theory of measures on infinite dimensional vector spaces (such as the space of initial conditions) has some subtleties, among which is the fact that well-defined measures should be probability measures (this means that \(\int_V d\mu = 1\)) [10]. A uniform measure would not have such property. It is convenient to digress a bit and introduce some basic concepts from measure theory. In the case of infinite dimensional vector spaces \(V\), there is an object, called the Fourier Transform of the measure \(\mu\). It is defined as

\[
\chi_\mu(f) := \int_V d\mu \, e^{i f(\varphi)},
\]

where \(f(\varphi)\) is an arbitrary continuous function(al) on \(V\). It turns out that under certain technical conditions, the Fourier transform \(\chi\) characterizes completely the measure \(\mu\). This fact is particularly useful for us since it allows to give a precise definition of a Gaussian measure. Let us assume that \(V\) is a Hilbert space and \(B\) a positive-definite, self-adjoint operator on \(V\). Then a measure \(\mu\) is said to be Gaussian if its Fourier transform has the form,

\[
\chi_\mu(f) = \exp \left( -\frac{1}{2} \langle f, B f \rangle_V \right),
\]

where \(\langle \cdot, \cdot \rangle_V\) is the Hermitian inner product on \(V\). We can, of course, ask what the measure \(\mu\) looks like. The answer is that, schematically it has the form,

\[
“d\mu = \exp \left( -\frac{1}{2} \langle \varphi, B^{-1} \varphi \rangle_V \right) D\varphi”,
\]

where \(D\varphi\) represents the fictitious “Lebesgue-like” measure on \(V\). The expression \(\langle \cdot, \cdot \rangle_V\) should be taken with a grain of salt since it is not completely well defined (whereas \(\langle \cdot, \cdot \rangle\) is). It is nevertheless useful for understanding where the denomination of Gaussian comes from. This can be seen from the term \(-\frac{1}{2} \langle \varphi, B^{-1} \varphi \rangle_V\) that is (finite and) negative definite, thus endowing \(\mu\) with its Gaussian character.

Let us return to the previous discussion regarding the representation of the CCR. We have argued that the trivial representation, given by a “uniform measure” is non-existent, and furthermore one is forced to consider a probabilistic measure. Notice that other than being a probabilistic measure, we have no further restrictions on what the measure \(\mu\) should be. It is a part of “folklore”, in the theoretical physics community, that the correct measure for our case is Gaussian. It is precisely one of the purposes of this article to motivate and illustrate this widely known result. Therefore, we shall try to take the most straight logical path to the desired result. What we need to do is to find the measure \(\mu_F\) that corresponds to the Fock representation. That is, given a Fock Hilbert space \(\mathcal{H}_F\), we want to find the Schrödinger Hilbert space that is “equivalent” to it. So far, we have not been precise about what we mean by
being equivalent. Once we use the proper setting for specifying “equivalence” of Hilbert spaces the right measure will be straightforward to find.

Let us summarize our situation. We saw that in order to construct the Fock quantum theory, in addition to the naturally defined symplectic structure on phase space, we needed to specify an additional classical structure, namely a complex structure $J$ on phase space. Furthermore, we have concluded that we need to specify a measure on the function space $V$ for the Schrödinger representation. The natural strategy is then to try to use the information that the complex structure $J$ provides, and employ it for finding the correct measure. We will see in the next section that $J$ provides us with precisely the right structure needed for the quantum equivalence notion that the Algebraic Formulation of Quantum Field Theory defines.

**B. Algebras and States**

The question we want to address is how to formulate equivalence between the two representations, namely Fock and Schrödinger for the scalar field theory. The most natural way to define this notion is through the algebraic formulation of QFT (see [4] and [6] for introductions). The main idea is to formulate the quantum theory in such a way that the observables become the relevant objects and the quantum states are “secondary”. Now, the states are taken to “act” on operators to produce numbers. For concreteness, let us recall the basic constructions needed.

The main ingredients in the algebraic formulation are two, namely: (1) a $C^*$-algebra $A$ of observables, and (2) states $\omega : A \to \mathbb{C}$, which are positive linear functionals ($\omega(A^*A) \geq 0 \forall A \in A$) such that $\omega(1) = 1$. The value of the state $\omega$ acting on the observable $A$ can be interpreted as the expectation value of the operator $A$ on the state $\omega$, i.e. $\langle A \rangle = \omega(A)$.

For the case of a linear theory, the algebra one considers is the so-called Weyl algebra. Each generator $W(\lambda)$ of the Weyl algebra is the “exponentiated” version of the linear observables, labeled by a phase space vector $\lambda^a$. These generators satisfy the Weyl relations:

$$W(\lambda)^{*} = W(-\lambda), \quad W(\lambda_1)W(\lambda_2) = e^{i\Omega(\lambda_1, \lambda_2)}W(\lambda_1 + \lambda_2).$$

(4.8)

The CCR get now replaced by the quantum Weyl relations where now the operators $\hat{W}(\lambda)$ belong to the (abstract) algebra $A$. Quantization in the old sense means a representation of the Weyl relations on a Hilbert space. The relation between these concepts and the algebraic construct is given through the GNS construction that can be stated as the following theorem [9]:

Let $A$ be a $C^*$-algebra with unit and let $\omega : A \to \mathbb{C}$ be a state. Then there exist a Hilbert space $\mathcal{H}$, a representation $\pi : A \to \mathcal{L}(\mathcal{H})$ and a vector $|\Psi_0\rangle \in \mathcal{H}$ such that,

$$\omega(A) = \langle \Psi_0, \pi(A)\Psi_0 \rangle_{\mathcal{H}}.$$ 

(4.9)

Furthermore, the vector $|\Psi_0\rangle$ is cyclic. The triplet $(\mathcal{H}, \pi, |\Psi_0\rangle)$ with these properties is unique (up to unitary equivalence).

One key aspect of this theorem is that one may have different, but unitarily equivalent, representations of the Weyl algebra, which will yield equivalent quantum theories. This is the precise sense in which the Fock and Schrödinger representations are related to each other. Let us be more specific. We have in previous sections constructed a Fock representation of the CCR, with the specification of a complex structure $J$. Using this representation, we can now compute the expectation value of the Weyl operators on the Fock vacuum and thus obtain a positive linear functional $\omega_{\text{fock}}$ on the algebra $A$. Now, the Schrödinger representation that will be equivalent to the Fock construction will be the one that the GNS construction provides for the same algebraic state $\omega_{\text{fock}}$. Our job now is to complete the Schrödinger construction such that the expectation value of the corresponding Weyl operators coincide with those of the Fock representation.

The first step in this construction consists in writing the expectation value of the Weyl operators in the Fock representation in terms of the complex structure $J$. The action of the state $\omega_{\text{fock}}$ on the Weyl algebra elements $\hat{W}(\lambda)$ is given by [9, 11, 18]

$$\omega_{\text{fock}}(\hat{W}(\lambda)) = e^{-\frac{i}{2}\mu(\lambda, \lambda)},$$

(4.10)

where $\mu(\cdot, \cdot) := \Omega(J\cdot, \cdot)$ is the positive definite metric defined on the phase space.
C. Measure and Representation

The next step is to complete the Schrödinger representation, which is now a two step process. First we need to find the measure \( d\mu \) on the quantum configuration space in order to get the Hilbert space \((\Sigma, \langle \cdot, \cdot \rangle)\) and second we need to find the representation \((\lambda^\alpha, \Phi_\alpha)\) of the basic operators.

Let us write the complex structure \( J \) in terms of the initial data. On the phase space \((\Gamma, \Omega)\) with coordinates \((\phi, \pi)\), the most general form of the complex structure \( J \) is given by

\[
-J_\Gamma(\phi, \pi) = (A\phi + B\pi, C\pi + D\phi),
\]

where \(A, B, C\) and \(D\) are linear operators satisfying the following relations \([20]\):

\[
A^2 + BD = -1, \quad C^2 + DB = -1, \quad AB + BC = 0, \quad DA + CD = 0.
\]

The inner product \( \mu(\cdot, \cdot) = \Omega(\cdot, -J_\Gamma \cdot) \) in terms of these operators is given by

\[
\mu((\phi_1, \pi_1), (\phi_2, \pi_2)) = \int_\Sigma d^3x (\pi_1 B\pi_2 + \pi_1 A\phi_2 - \phi_1 D\phi_2 - \phi_1 C\pi_2),
\]

for all pairs \((\phi_1, \pi_1)\) and \((\phi_2, \pi_2)\) in \(\Gamma\). As \(\mu_\Gamma\) is symmetric and positive definite, then the linear operators should also satisfy \([20]\)

\[
\int_\Sigma fBf' = \int_\Sigma f'Bf, \quad \int_\Sigma gDg' = \int_\Sigma g'Dg, \quad \int_\Sigma fAg = -\int_\Sigma gCf,
\]

and

\[
\int_\Sigma fBf' > 0, \quad \int_\Sigma gDg' < 0,
\]

for all scalars \(g, g' \in C^\infty_0(\Sigma)\) and unit weight scalars densities \(f, f' \in C^\infty_0(\Sigma)\).

With this in hand, we can find the measure \( d\mu \) that defines the Hilbert space. In order to do this, it suffices to consider configuration observables. That is, we shall consider observables of the form \(\phi[f] = \int d^3x f \phi\), which correspond to a vector of the form \(\lambda^\alpha = (0, f)^\alpha\). Now, we know how to represent these observables independently \((\lambda^\alpha, \Phi_\alpha)\) as given by \((4.3)\). In the Schrödinger picture, the Weyl observable \(\hat{W}(\alpha)\) with label \(\lambda^\alpha = (0, f)^\alpha\) has the form

\[
\hat{W}_{\text{sch}}(\lambda) = e^{\hat{\phi}[f]}.
\]

Now, the equation \((4.10)\) tells us that the state \(\omega_{\text{sch}}\) should be such that

\[
\omega_{\text{sch}}(\hat{W}(\lambda)) = \exp \left[ -\frac{1}{4} \int_\Sigma d^3x fBf \right],
\]

where we have used the inner product \((4.13)\). On the other hand, the left hand side of \((4.10)\) is the vacuum expectation value of the \(\hat{W}(\lambda)\) operator. That is,

\[
\omega_{\text{sch}}(\hat{W}(\lambda)) = \int_{\Sigma} d\mu \Psi_0(\hat{W}_{\text{sch}}(\lambda) \cdot \Psi_0) = \int_{\Sigma} d\mu e^{i \int_\Sigma d^3x f \phi}.
\]

Let us now compare \((4.17)\) and \((4.18)\),

\[
\int_{\Sigma} d\mu e^{i \int_\Sigma d^3x f \phi} = \exp \left[ -\frac{1}{4} \int_\Sigma d^3x fBf \right].
\]

Let us now recall our previous discussion regarding the Fourier transform of a Gaussian measure, given by Eq. \((4.6)\). Then we note that \((4.19)\) tells us that the measure \(d\mu\) is Gaussian and that it corresponds heuristically to a measure of the form

\[
"d\mu = e^{-\int_\Sigma \varphi B^{-1} \varphi D\varphi".}
\]
This is the desired measure. However, we still need to find the “multiplicative term” in the representation of the momentum operator (4.4). For that, we will need the full Weyl algebra and Eq. (4.10). Let us write the most general momentum operator as \((\hbar = 1)\),
\[
(\hat{\pi}[g] \cdot \Psi)[\varphi] = -i \int_\Sigma \left( g \frac{\delta}{\delta \varphi} \right) \Psi[\varphi] + \hat{M} \cdot \Psi[\varphi].
\]
(4.21)

Imposing (4.10) and using the Baker-Campbell-Hausdorff (BCH) relation, it can be shown that the momentum operator is uniquely given by the expression [18]
\[
(\hat{\pi}[g] \cdot \Psi)[\varphi] = -i \int_\Sigma \left( g \frac{\delta}{\delta \varphi} - \varphi (B^{-1} - iCB^{-1}) g \right) \Psi[\varphi],
\]
(4.22)
which explicitly exhibits the form of the multiplicative term.

To summarize, we have used the vacuum expectation value condition (4.10) in order to construct the desired Schrödinger representation, namely, a unitarily equivalent representation of the CCR on the Hilbert space defined by functionals of initial conditions. We have provided the most general expression for the quantum Schrödinger theory, for arbitrary embedding of \(\Sigma\) into \(4M\). From the discussion of Sec. IV A, we saw that the only possible representation was in terms of a probability measure, thus ruling out the naive “homogeneous measure”. This conclusion made us realize that both the choice of measure and the representation of the momentum operator were intertwined; the information about the complex structure \(J\) that lead to the “one-particle Hilbert space” had to be encoded in both of them. We have shown that the most natural way to put this information as conditions on the Schrödinger representation was through the condition (4.10) on the vacuum expectation values of the basic operators. This is the non-trivial input in the construction.

Several remarks are in order.

1. In Sec. IV A we made the distinction between the classical configuration space \(C\) of initial configurations \(\varphi(x)\) of compact support and the quantum configuration space \(\overline{C}\). So far we have not specified \(\overline{C}\). In the case of flat embeddings, where \(\Sigma\) is a Euclidean space, the quantum configuration space is the space \(J^*\) of tempered distributions on \(\Sigma\). However, in order to define this space one uses the linear and Euclidean structure of \(\Sigma\) and it is not trivial to generalize it to general curved manifolds. This subtleties lie outside the scope of this paper, and will be reported elsewhere [21].

2. Note that the form of the measure given by (4.19) is always Gaussian. This is guarantied by the fact that the operator \(B\) is positive definite in the ordinary \(L^2\) norm on \(\Sigma\), whose proof is given in [20]. However, the particular realization of the operator \(B\) will be different for different embeddings \(T_i\) of \(\Sigma\). Thus, for a given \(J\), the explicit form of the Schrödinger representation depends, of course, on the choice of embedding.

3. In the discussion regarding quantization in section II, we saw that the operator \(\hat{\pi}[g]\) should be Hermitian. It is straightforward to show that the operator given by (4.22) indeed satisfies this requirement.

4. The last term in the representation of the momentum operator containing the \(C\) operator, is somewhat unexpected; it can not be guessed from the form of the measure, that knows only about \(B\). One might hope that one can get rid of this term by a suitable canonical transformation. However, it has been shown that the absence of this term in the momentum operator (i.e. same \(B\) and \(C = 0\)) might lead to inequivalent quantum theories [23], and examples of such cases have been explicitly constructed [24].

5. Note that the presence of \(B\) and \(C\) in the momentum operator (4.22) emphasize the ambiguity inherent in field theory. However, for a scalar field propagating on a Minkowski background there is one preferred complex structure (namely, that one selected by requiring Poincaré invariance) and hence a preferred Schrödinger representation. We shall come back to this issue in later sections.

6. We have mentioned in the previous discussion that one can alternatively interpret the quantization ambiguity in the choice of different vacua. In the [23] these vacua are constructed in the general case. It is shown that they are closely related to the measure, but also know about the extra information, namely the operator \(C\).

In previous sections we have successfully answered the question of finding a Schrödinger representation unitarily equivalent to a given Fock representation. However, the precise relation between them, i.e. a mapping between states is still missing. That is the purpose of the following section.
V. FROM FOCK TO SCHRÖDINGER

The question we want to address is how the two representations are related, and how can we pass from one to the other. Let us consider the simplest case which is the passage from the Fock representation to the Schrödinger. We begin with the preferred, cyclic state, namely the vacuum $|0\rangle$. Let us denote by ‘Kets’ the elements of the abstract Hilbert space of states, and use the brackets for states in some representation. Then $\langle \varphi|0\rangle$ represents the vacuum in the Schrödinger representation. Let us denote by $(\bar{n}|0\rangle$ the vacuum in the Fock representation, using a notation in analogy to the $n$-particle states of, say, a harmonic oscillator.

The first step in this direction is to assume that we have the Fock states, and both representations. Then, our strategy will be the following: represent the creation and annihilation operators acting on wave functionals. If we manage to do this we would be able to have a way of converting a Fock state into a Schrödinger state. For, almost all states on the Fock space can be generated by acting, with suitable creation operators on the vacuum. Thus, by acting on the Schrödinger vacuum we would be able to create a dense subset of states. This strategy assumes that we know what the vacuum in the Schrödinger representation is. From the discussion in Sec. [Sec. IV A] we know that the Schrödinger vacuum $\langle \varphi|0\rangle$ is given (up to a constant phase) by the constant function

$$\Psi_0(\varphi) := \langle \varphi|0\rangle = 1. \quad (5.1)$$

The next step is to represent creation and annihilation operators on $\mathcal{H}_\varphi$. This is given by the following expression. If we represent by $\zeta^a = (-g,f) \in \Gamma$ a label-vector in the phase space, we can define the corresponding observable $O_\zeta = \varphi[f] + \pi[g]$ and therefore, a quantum observable $\hat{O}(\zeta)$. We can now recover the creation and annihilation operators as follows,

$$C(\zeta) := \frac{1}{2\hbar}(\hat{O}(J\zeta) + i\hat{O}(\zeta)) \quad (5.2)$$

and

$$A(\zeta) := \frac{1}{2\hbar}(\hat{O}(J\zeta) - i\hat{O}(\zeta)). \quad (5.3)$$

Recall that the complex structure $J$ acts on initial data as $-J(\varphi,\pi) = (A\varphi + B\pi, C\pi + D\varphi)$. Then we have,

$$C(-g,f) = \frac{1}{2\hbar}(\hat{\varphi}[Dg - Cf + if] + \hat{\pi}[Bf - Ag + ig]). \quad (5.4)$$

The annihilation operator can be written in a similar way,

$$A(-g,f) = \frac{1}{2\hbar}(\hat{\varphi}[Dg - Cf - if] + \hat{\pi}[Bf - Ag - ig]). \quad (5.5)$$

These expressions (5.4) and (5.5) are completely general, for any $J$ and any representation. In the particular case we are interested, namely when the representation is equivalent to the Fock one and is given by (4.3) and (4.22), then we have the desired operators. Note that in order to have a consistent formulation we should have that

$$A(-g,f) \cdot \Psi_0[\varphi] = 0, \quad (5.6)$$

for all $f$ and $g$. It is straightforward to check that this is indeed the case.

We can also find the “one-particle state” in the Schrödinger representation, which we will denote by $\Phi_\zeta^1 := C[\zeta] \cdot \Psi_0$. Using the creation operator (5.4) on the vacuum state we have that

$$\Phi_\zeta^1[\varphi] = \frac{i}{\hbar} \left( \int d^3x \, \varphi[f + i(B^{-1} - iC^{-1})g] \right) \quad (5.7)$$

is the “one particle state” given by the vector $\zeta = (-g, f)$. Furthermore, any state in the Schrödinger representation can be obtained by successively acting with the creation operator (5.4).

In the functional picture the two-point function corresponds to the $L^2(\mathcal{C}, d\mu)$-inner product between the “one-particle” Schrödinger states $\Phi_\zeta^1(\varphi)$ and $\Phi_\eta^1(\varphi)$,

$$\langle \Phi_\zeta^1(\varphi), \Phi_\eta^1(\varphi) \rangle = \bar{\zeta}A\eta^A = \frac{1}{2\hbar} \mu(\zeta, \eta) - \frac{i}{2\hbar} \Omega(\zeta, \eta). \quad (5.8)$$
More precisely, the specification of an algebraic state \( \omega \) corresponds to the specification of all the smeared \( n \)-point functions of the quantum field. In particular, the two-point function of the quantum field in the state \( \omega \) is defined by

\[
\langle \hat{O}(\zeta)\hat{O}(\eta) \rangle_\omega = -\frac{\partial^2}{\partial s \partial t} \omega(\hat{W}(s\zeta + t\eta)) \exp(ist\Omega(\zeta, \eta)/2) |_{s=t=0},
\]

whereas the higher \( n \)-point functions of the quantum field are defined similarly by using the Weyl relations. Since \( \hat{O}(\xi) = i(A(\xi) - C(\xi)) \), it is straightforward to verify that the last definition gives (5.5) for the algebraic state (4.10). In terms of configuration and momentum operators the two-point function (5.5) can be written explicitly as follows (with \( \zeta = (-g_1, f_1) \) and \( \eta = (-g_2, f_2) \)):

\[
\langle \Phi^\dagger_{\xi}(\phi), \Phi^\dagger_{\eta}(\phi) \rangle = \langle \Psi_0, \phi[f_1]\phi[f_2]\Psi_0 \rangle + i\langle \Psi_0, \phi[f_1]\phi[(1-iC)B^{-1}g_2]\Psi_0 \rangle + i\langle \Psi_0, \hat{\pi}[g_1]\phi[(1-iC)B^{-1}g_2]\Psi_0 \rangle + \langle \Psi_0, \hat{\pi}[g_1]\phi[f_2]\Psi_0 \rangle.
\]

Thus, the second moment of the measure \( d\mu \), that corresponds to the choice \( \zeta = \eta = (0, f) \), is given by

\[
\langle \Psi_0, \phi[f]^2\Psi_0 \rangle = \int C d\mu \phi[f]^2 = \frac{1}{2} \int f^3 Bf.
\]

In general, the \( n \)-th moment of the quantum measure goes as the \( n/2 \) power of the covariance (two-point function of \( d\mu \) )

\[
\int C d\mu \phi[f]^n = c_n \left( \frac{1}{2} \int fBf \right)^{n/2},
\]

where \( c_n \) is a constant. Thus, as we expect from the previous discussion (section VI.4.4), the whole properties of the measure will be dependent of those satisfied by \( B \).

Let us now comment on the reverse question, namely how to find the corresponding Fock state, given a state in the functional representation. This problem is more involved. Let us recall what happens in the case of a harmonic oscillator. In that case, the “Fock representation” is given by the states expanded on the basis of the form \( \langle n|\psi \rangle \), and the corresponding image of the basis states are the Hermite polynomials \( H_n(q) \) in the Schrödinger picture. Now, given a state \( \psi(q) \), one can always decompose it in the basis given by the Hermite polynomials \( \psi(q) = \sum_n a_n H_n(q) \), then the corresponding state in the Fock picture is given by \( |\psi\rangle = \sum_n a_n |n\rangle \). That is, the state is given by the array of coefficients \( (a_0, a_1, \ldots, a_n, \ldots) \) in the (Hermite) expansion. In the case of the field theory, given any Schrödinger state, one would have to decompose it in a “Hermite expansion” in order to find its corresponding state in the Fock picture. We will not attempt to do so in this paper. Note that this can indeed be done when the representation is complex analytic, a la Bargmann, as done in [24].

VI. EXAMPLES

We have stated that there are infinite inequivalent representations of the CCR. The structure responsible for this fact can be taken as the complex structure \( J \). In the Fock representation, it is responsible for the separation of the space of solutions into ‘positive’ and ‘negative’ frequency solutions (to follow the standard terminology), which gives meaning to the notion of particle. In the Schrödinger representation the complex structure manifests itself in the space of solutions into ‘positive’ and ‘negative’ frequency solutions (to follow the standard terminology), which
the existence of a natural ‘time dependent’ complex structure. Naturally, Minkowski spacetime possesses a sphere’s worth of such vector fields (one for each global inertial observer). A natural question one might ask is how the two requirements are connected. That is, Can the requirement of Poincaré invariance be compatible with the natural construction from the Killing fields? Is there a unique choice satisfying both conditions? As we shall see the answers are in the affirmative.

In this section we shall consider concrete examples of spacetimes in which the quantum field theory is constructed. The remainder of this section has three parts. In the first one, we shall review the standard construction of the quantum field theory in rigid Minkowski spacetime. A novel and the functional representation has not appeared before. In the second part we shall consider stationary spacetimes and in the last one, some simple cosmological solutions such as Robertson-Walker spacetimes. Even when these examples have been considered elsewhere, the approach taken here is novel and the functional representation has not appeared before.

A. Minkowski Spacetime

Let us consider any two inertial observers $O_1$ and $O_2$ in $(M, \eta_{ab})$. The coordinate system of each observer corresponds to spacetime foliations that define timelike Killing vector fields $t^1_2$ and $t^2_2$, respectively. The spacelike Cauchy surfaces $T_{t_1}(\Sigma)$ are chosen to be the (unique) normal to $t^1_2$ (for $i = 1, 2$), namely the inertial frame in which the vector field $t^1_2$ is “at rest”. The observers $O_1$ and $O_2$ decomposes solutions in its positive and negative frequency parts with respect to the associated Killing vector field, defining in such a way the $(\Omega)$-compatible complex structures $J_1 = -(L_{t_1}L_{t_1})^{-1/2}L_{t_1}$ and $J_2 = -(L_{t_2}L_{t_2})^{-1/2}L_{t_2}$. In general, every inertial observer defines a complex structure of the type $J = -(L_{\xi}\xi)^{-1/2}\xi$, where the vector field $\xi$ in $TM$ coincides with $(\partial/\partial t)^a$ in the observer coordinate system $X : M \to \mathbb{R}^4, p \mapsto X(p) = (t, x, y, z)$.

Now, since $O_1$ and $O_2$ are inertial observers, they are related by a Poincaré transformation $P$ which in turn induces a transformation on the covariant phase space $\Gamma_S$. From the one parameter family of embeddings $T_i$, we will choose $T := T_{i=0}$ to be the embedding from which the canonical version of the theory will be constructed. The (active) Poincaré transformation maps every Cauchy surface $T_i(\Sigma)$ onto Cauchy surfaces $T_{\bar{t}_i}(\Sigma) = P(T_i(\Sigma))$ that corresponds to equal time surfaces for $O_2$. Thus, in particular, we have that $T'(\Sigma) = P(T(\Sigma))$ and therefore the corresponding Cauchy data associated to a solution $\phi$ of the Klein-Gordon equation are different; namely, $\varphi(x) = (\phi \circ T)(x)$ and $\pi(x) = \sqrt{\eta}_{\nu\alpha}(\phi \circ T)(x)$ are the Cauchy data with respect to the embedding $T$, whereas $\varphi'(x) = (\phi \circ T')(x)$ and $\pi'(x) = \sqrt{\eta}_{\nu\alpha}(\phi \circ T')(x)$ are the corresponding Cauchy data with respect to $T'$. Hence, it is clear that the (active) Poincaré transformation $P : M \to M$ induces on the space of solutions, via $T' = P \circ T$, the transformation $\phi \to \phi' = P^*\phi$. This symplectic transformation $P^* : \Gamma_S \to \Gamma_S$ in turn induces a $(\Omega)$-compatible complex structure $J' = P^*J_1P^*-1$. Indeed,

$$\mu_1(\phi, \phi) = \Omega(J_1\phi, \phi) = \Omega(P^*J_1P^*-1\phi', \phi') =: \mu'(\phi', \phi').$$

Now, while on the one hand we have a natural complex structure associated with the second observer, namely $J_2 = -(L_{t_2}L_{t_2})^{-1/2}L_{t_2}$, on the other hand we have an induced complex structure $J' = P^*J_1P^*-1$. Are these complex structures related? Are they equivalent? It turns out that the answer is in the affirmative; in fact these complex structures are exactly the same. In order to see this, let us consider the Poincaré transformation $P$ that induces a transformation $P_T$ such that the image of the vector $t^2_2$ “anchored” on $p \in T(\Sigma)$ is $t^2_2$ “anchored” on $p' = P : p \in T'(\Sigma)$. It is straightforward to verify (by using the mode decomposition of the field) that the operator $\Theta(t^2_2) := (L_{t_2}L_{t_2})^{-1/2}L_{t_2}$ satisfies $P^*\Theta(P_T^{-1}t^2_2)P^*-1 = \Theta(t^2_2)$. Then,

$$-J_2 = -(L_{t_2}L_{t_2})^{-1/2}L_{t_2} = (L_{P_Tt_1}L_{P_Tt_1})^{-1/2}L_{P_Tt_1} = P^*(L_{t_1}L_{t_1})^{-1/2}L_{t_1}P^{-1} = -J'.\quad (6.1)$$

That is to say, the natural complex structure associated to an inertial frame is covariant under the Poincaré group. Moreover, it is easy to see that given a positive (negative) frequency solution $\phi^+$ ($\phi^-$) with respect to $t^1_2$ and $J_1$, $J_2\phi^+ = i\phi^+$ ($J_2\phi^- = -i\phi^-$) and therefore $J_1\phi = J_2\phi$. Since $J_2 = P^*J_1P^*-1$, then $(P^*J_1 - J_1P^*)\phi = 0$; i.e., the natural complex structure $J = -\Theta(t^2)$ is invariant under Poincaré transformations (furthermore, $J$ is unique since it satisfies $\Omega(JL_\xi\phi, \phi) = 0$ [24]) and consequently $P$ will be unitary relative to the complex pre-Hilbert structure

\[^{2}\text{We say that } J \text{ is invariant relative to a given symplectic group if it commutes with all the symplectic transformations in the group. If the}]

\[\]
(ΓS, μ = Ω(J)). To summarize, we have proved that the usual positive-negative frequency decomposition found everywhere is indeed the unique complex structure that is Poincaré invariant.

The Poincaré invariant complex structure on ΓS, J = −Θt^a, has a counterpart J_F on the Cauchy data space, provided by the (embedding-dependent) isomorphism I_T : Γ → ΓS through J_F = I_T^{-1}J_I T. This relation and the general form (4.11) implies that

\[ A\varphi + B\pi = -T^a[J\phi], \quad C\pi + D\varphi = -T^a[\sqrt{h}E_a(J\phi)]. \quad (6.2) \]

If T represents an “inertial embedding” of R^3 into M, it is not difficult to see that the complex structure J_F is given by \( J_F(\varphi, \pi) = ((-\Delta + m^2)^{-1/2}\pi, (\Delta + m^2)^{-1/2}\varphi) \), which means that \( A = C = 0, B = (-\Delta + m^2)^{-1/2} \) and \( D = (\Delta + m^2)^{1/2} \). The quantum measure is then \( \text{d}\mu = e^{-\int \sqrt{h}(\Delta + m^2)^{1/2}\sqrt{g}\,D\varphi} \). Thus, we obtain the Gaussian measure and Fock representations existing in the literature [3, 4, 26]. As should be clear from the discussion, this represents a very particular case of the general formulae presented above. The momentum operator (4.22) is given by

\[ (\hat{\pi}[g], \Psi)[\varphi] = -i \int_{R^3} d^3x \left( g \frac{\delta}{\delta \varphi} - \varphi (\Delta + m^2)^{1/2} g \right) \Psi[\varphi], \]

and provides us with a preferred representation in the sense that it arose by requiring Poincaré invariance.

### B. Stationary Spacetimes

We shall consider here spacetimes which possess a timelike Killing vector field t^a and such that a spacelike hypersurface, orthogonal to the orbits of the isometry, might not exist. In particular, the Killing vector field provides us with a natural slicing of spacetime into space and time, and the shift function necessarily will be different from zero, when the vector field is not hypersurface orthogonal.

Now, it is well-known [20, 27, 28] that given a real Hilbert space \( \mathcal{H} \) and a non degenerate symplectic structure defined thereon, then there exists a complex structure \( J \) on \( \mathcal{H} \) and a real scalar product \( \mu \) such that \( \Omega(x, y) = \mu(Jx, y) \). Indeed, by the Riesz lemma there exists a continuous linear operator \( E : \mathcal{H} \to \mathcal{H} \) such that \( \Omega(x, y) = \langle Ex, y \rangle \), where \( \langle \cdot, \cdot \rangle \) denotes the given scalar product on \( \mathcal{H} \). Since the complex structure is skew, then \( E^* = -E \) and \( -E^2 \geq 0 \). It is not difficult to see that \(-E^2\) is a continuous linear operator and therefore there is (by the square root lemma [17]) a unique bounded operator \( |E| \) with \( |E| \geq 0 \) and \( |E| = \sqrt{-E^2} \). Moreover, it can be shown that \( |E| \) is self-adjoint injective, has a dense range and an inverse \( |E|^{-1} \). From the polar decomposition theorem [17], since \( E \) is a bounded linear operator on \( \mathcal{H} \), there is a partial isometry \( U \) such that \( |E|U = E \). This partial isometry defines a complex structure \( J = |E|^{-1}E \), \( -E^2 = |E|^2 \) implies \( J^2 = -1 \) and is orthogonal \( J^* = -J = J^{-1} \). Hence, the scalar product \( \mu \) on \( \mathcal{H} \) is defined by

\[ \mu(x, y) = \langle |E|x, y \rangle. \]

Let \( F \) be the operator that dictates classical evolution in the canonical framework. The idea is to prescribe the inner product on the Cauchy data space \( \Gamma \) as \( \langle F^a, \cdot, \cdot \rangle = \Omega(\cdot, \cdot) \), in such a way that \( F \) will be an anti-self-adjoint operator and hence \(-F^2\) will be non-negative. From the Klein-Gordon Hamiltonian

\[ H_{KG} = \frac{1}{2} \int_{\Sigma} d^3x \sqrt{h} \left( \frac{N^a}{h} \dot{\varphi}^2 + Nh^{ab}D_a\varphi D_b\varphi + Nm^2\varphi^2 + \frac{2\pi}{\sqrt{h}} N^a D_a\varphi \right), \quad (6.4) \]

it is easy to see that the equations of motion are given by

\[ \left( \begin{array}{c} \dot{\varphi} \\ \pi \end{array} \right) = \left( \begin{array}{c} F \\ \pi \end{array} \right), \quad \text{where} \quad F = \left( \begin{array}{cc} N^a D_a & N \\ -\Theta & \Lambda \end{array} \right) \quad (6.5) \]

and \( \Theta := -\sqrt{h}(ND_a D_a + D^a ND_a - Nm^2), \Lambda := \sqrt{h}D_a(N^a) + N^a D_a) \), \( N := N/\sqrt{h}, N^a := N^a/\sqrt{h} \). From \( \Omega((\varphi_1, \pi_1), (\varphi_2, \pi_2)) = \Omega(F(\varphi_1, \pi_1), (\varphi_2, \pi_2)) \) it is clear that \( F^* = -F \) indeed, and consequently there is a unique \(|F|\), non-negative, that satisfies

\[ |F||F| = -F^2. \quad (6.6) \]

complex structure is invariant under a given symplectic transformation \( T \) on \( \Gamma_S, T \) will be unitary relative to the complex pre-Hilbert structure provided by [3, 4, 26].
Let $|F|$ be the matrix
\[ |F| = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \] (6.7)
since $|F|$ is self adjoint, then the operators $a, b, c$ and $d$ must be such that
\[ \int \varphi d\pi = \int \varphi d\pi, \quad \int \varphi_1 \varphi_2 = -\int \varphi_2 \varphi_1, \quad \int \pi_1 b \pi_2 = -\int \pi_2 b \pi_1. \] (6.8)
Now, the relationship (6.6) implies the following system of operator equations that one has to solve in order to find the general expression for the complex structure $J$,
\[ a^2 + bc = N\Theta - N^a D_a N^b D_b. \] (6.9)
\[ ab + bd = -(N^a D_a N + N\Lambda). \] (6.10)
\[ ca + dc = \Theta N^a D_a + \Lambda \Theta. \] (6.11)
\[ cb + d^2 = \Theta N - \Lambda^2. \] (6.12)
Note that if we restrict our attention to orthogonal foliations (which in turn are natural for static spacetimes) then we recover the particular case specified in the appendix of [20] by Ashtekar and Magnon (with slight differences that come from the fact that, instead of scalars, here the momenta are scalars densities of weight one). Indeed, if $N^a = 0$, then (6.9)-(6.12) yields
\[ a^2 + bc = N\Theta, \quad ab + bd = ac + dc = 0, \quad cb + d^2 = \Theta N, \] (6.13)
which means that $a = (N\Theta)^{1/2}$, $d = (\Theta N)^{1/2}$, and $b = c = 0$. Therefore
\[ |F|^{-1} = \begin{pmatrix} (N\Theta)^{-1/2} & 0 \\ 0 & (\Theta N)^{-1/2} \end{pmatrix}, \] and the complex structure that one obtains by virtue of the polar decomposition is
\[ J = \begin{pmatrix} 0 & \Theta^{-1/2} N^{1/2} \\ -N^{-1/2} \Theta^{1/2} & 0 \end{pmatrix}, \] (6.14)
that is to say $B = \Theta^{-1/2} N^{1/2}$, $D = -N^{-1/2} \Theta^{1/2}$ and $A = C = 0$ (c.f. eq. 4.11).
Thus, the requirements in the appendix of [20] are equivalent to perform the polar decomposition by using the infinitesimal evolution operator associated to the Hamiltonian density
\[ \mathcal{H}_{KG} = \frac{N\sqrt{h}}{2} \left( \frac{\pi^2}{\hbar} + D^a \varphi D_a \varphi + m^2 \varphi^2 \right). \]
In this particular case, the form of the measure is
\[ "d\mu = e^{-\int \varphi (N^{-1/2} \Theta^{1/2} \varphi) D \varphi"}, \]
Let us end our detour into orthogonal foliations and return to the more general case where $b$ and $c$ will be different from zero, and hence with non zero shift (i.e., $N^a \neq 0$). If this is the case, the operators that one obtains via the polar decomposition, and that specify the complex structure (4.11), are given by
\[ A = \Upsilon N^a D_a - d\Theta, \quad B = \Upsilon N + \Delta \Lambda, \]
\[ C = -d^{-1} c \Upsilon N - b^{-1} a \Delta \Lambda, \quad D = b^{-1} a \Delta \Theta - d^{-1} c \Upsilon N^a D_a, \] (6.15)
where $\Delta := (c-db^{-1}a)^{-1}$ and $\Upsilon := (a-bd^{-1}c)^{-1}$. This complex structure on the Cauchy data space $\Gamma$ corresponds to the (negative of the) complex structure induced by the covariant one $J = (-L_t, L_t)^{-1/2}L_t$ that is the unique complex structure that satisfies the energy-requirement, as Ashtekar and Magnon showed \cite{20, 21}. More precisely, let $T_t$ be the uniparametric family of embeddings of $\Sigma$ into $M$ that corresponds to a slicing with respect to the timelike Killing vector field $t^\alpha$, then the induced complex structure on $\Gamma$ is given by $I_T^{-1}(-L_t, L_t)^{-1/2}L_t IT$, where $I_T : \Gamma \to \Gamma_\Sigma$ is the natural isomorphism (associated to an embedding $T$ of the family) between the space of Cauchy data and the space of solutions. Thus, $F = I_T^{-1}L_t IT$ and $|F|^{-1} = I_T^{-1}(-L_t, L_t)^{-1/2}IT$.

The quantum measure is then

$$ “d\mu = e^{-\int \varphi(\Upsilon N + \Delta) - 1/2} D\varphi”, $$

and the preferred representation for the momentum operator \cite{6, 22}, selected by the energy-requirement, is given by

$$ (\hat{\pi}[\varphi] \Psi)[\varphi] = -i \int_\Sigma d^3x \left\{ \frac{\delta}{\delta \varphi} - \varphi [1 + i (d^{-1}c \Upsilon N + b^{-1}a \Delta \Lambda)](\Upsilon N + \Delta \Lambda)^{-1}g \right\} \Psi[\varphi]. \quad (6.16) $$

### C. Cosmological Solutions

Let us consider now the Robertson-Walker cosmological model of homogeneous and isotropic universes. That is to say, spacetimes which spatial geometry, restricted by the homogeneity and isotropy requirements, is that one of (a) a sphere, (b) flat Euclidean space, or (c) a hyperboloid. For this class of spacetimes, the four-dimensional metric $g_{ab}$ may be expressed as $g_{ab} = -u_{a}u_{b} + h_{ab}$, where $u^a$ are the tangents to the world line of isotropic observers, which are orthogonal to the $3-d$ homogeneous surfaces with metric $h_{ab}$. Thus, the line element for the three possible spatial geometries, described in spherical, Cartesian and hyperbolic coordinates, respectively, is given by

$$ ds^2 = -d\tau^2 + a^2(\tau) \left\{ \begin{array}{l}
d\psi^2 + \sin^2 \psi (d\theta^2 + \sin^2 \theta d\phi^2), \quad 0 \leq \psi \leq 2\pi \\
dx^2 + dy^2 + dz^2 \\
d\psi^2 + \sinh^2 \psi (d\theta^2 + \sin^2 \theta d\phi^2), \quad 0 \leq \psi < \infty
\end{array} \right. $$

where $a(\tau)$ is a positive function of the proper time $\tau$ of any of the isotropic observers.

Now, the world lines of the isotropic observers define a time-like hypersurface orthogonal unit vector field $(\partial/\partial \tau)^a$, which in turns determines canonically a complex structure of the form \cite{6.14} on the space of Cauchy data by virtue of the polar decomposition of $L_\tau$. Since the lapse function is equal to one, then $\Theta = -\sqrt{h}(D^a D_a - m^2)$ and hence the complex structure \cite{6.14} will be specified, for each one of the possible geometries, by

$$(D^a D_a, \mathcal{N}) = $$

$$ \left\{ \begin{array}{l}
\frac{1}{a^2}(\partial^2_\psi + 2 \cot \psi \partial_\psi) \quad + \frac{1}{a \sin^2 \psi}(\partial^2_\theta + \cot \theta \partial_\theta + \frac{1}{\sin^2 \theta} \partial^2_\phi), \quad 1/a^3 \sin^2 \psi \sin \theta \\
\frac{1}{a^2}(\partial^2_\tau + \partial^2_\theta + \partial^2_\phi), \quad 1/a^3 \\
\frac{1}{a^2}(\partial^2_\psi + 2 \coth \psi \partial_\psi) \quad + \frac{1}{a^2 \sinh^2 \psi}(\partial^2_\theta + \cot \theta \partial_\theta + \frac{1}{\sin^2 \theta} \partial^2_\phi), \quad 1/a^3 \sinh^2 \psi \sin \theta
\end{array} \right. $$

The presence of $a(\tau)$ in the complex structure, through $D^a D_a$ and $\mathcal{N}$, implies that it is a time-dependent complex structure for each (dust or radiation-filled) Robertson-Walker universe and hence the vacuum state is unstable. Indeed, let $T$ be the embedding (of $\Sigma$ into the spacetime) that corresponds to the “equal time” Cauchy surface $\tau = \tau_1$, and let $J_t$ be the complex structure defined by the pair $(D^a D_a, \mathcal{N})$ at $\tau = \tau_1$. Then, the covariant complex structure is given by $J = I_T J_t I_T^{-1}$, where $I_T : \Gamma \to \Gamma_\Sigma$ is the natural isomorphism associated to $T$. The vacuum expectation associated to the fictitious complex structure $J' = I_T J_2 I_T^{-1}$ is, in general, different from the vacuum expectation associated to $J$. The algebraic states certainly will be different functionals on the Weyl algebra and consequently the Fock spaces obtained via the GNS construction disagree.

Finally, let us consider the particular case of a dust-filled Robertson-Walker flat universe. The explicit form of the complex structure in this background is given by

$$ J = \begin{pmatrix}
0 & \frac{1}{a^2}(-\Delta + M^2)^{-1/2} \\
-a^2(-\Delta + M^2)^{1/2} & 0
\end{pmatrix}, \quad (6.17) $$
where $\Delta$ denotes the Laplacian operator in Cartesian coordinates, $a(\tau) = (9C/4)^{1/3}r^{2/3}$ (with $C = 8\pi\rho a^3/3$ a constant) and $M(\tau) := ma(\tau)$. Thus, the Gaussian measure and the momentum operator are

\[ \text{``}d\mu = e^{-\int d^3x a^2(-\Delta + M^2)^{1/2} \mathcal{D}\varphi}\text{''}, \]

and

\[ \hat{\pi}[g] \cdot \Psi[\varphi] = -i \int_{\Sigma} d^3x \left( g \frac{\delta}{\delta \varphi} - \varphi a^2(-\Delta + M^2)^{1/2} g \right) \Psi[\varphi]. \]

The static case $a = \text{constant}$ is, of course, the case of Minkowski space (c.f. eq(6.3)).

**VII. DISCUSSION**

The aim of this paper was to present in a self-contained manner the main steps necessary to construct the Fock and Schrödinger representations for a real Klein-Gordon field on Minkowski spacetime, for arbitrary embeddings of the “constant time hypersurface”. We first briefly reviewed the canonical quantization procedure, emphasizing the definitions of the classical objects such as phase space and observables of a scalar field which are needed for its quantization.

For the covariant Fock quantization we started from the phase space of classical solutions of the Klein-Gordon equation and constructed the corresponding one-particle Hilbert space. In this construction we emphasized the role of the complex structure $J$ as responsible for the infinite freedom in the choice of the quantum representation for the Fock Hilbert space (alternatively one can use the metric $\mu$ [6]).

In the functional Schrödinger representation we discussed in detail the role played by certain classical constructs. For instance we have, in addition to $J$, a second classical object, namely the choice of embedding $T$. We argued that it is necessary to consider a probabilistic measure instead of the naive Lebesgue measure which, in fact, does not exist in this case. We showed that the choice of complex structure $J$ and embedding $T$ was manifest at the level of the measure $d\mu$ and in the representation of the momentum operator. In connection with the Hilbert space needed for the functional representation we made the distinction between the classical $C$ and the quantum $\overline{C}$ configuration spaces, but we have not specified $\overline{C}$.

This problem lies beyond the scope of this paper, and shall be reported elsewhere [21].

In order to relate explicitly the Fock and Schrödinger representations we have used the algebraic formulation of quantum field theory, by means of the GNS construction. Finally, we have discussed the explicit mapping that relates the states in both representations, and provided several examples of such constructions.

In this paper, we have only considered the Schrödinger functional picture where states are functions of the (real) configuration variable $\varphi$, or as sometimes it is known, the ‘vertical polarization’. There are alternative functional representations that have been considered in the literature (see for instance Ref. [24]). This representation are however, the functional equivalence of the Bargmann representation in quantum mechanics, where states are holomorphic functions on phase space (i.e. the holomorphic polarization), with complex coordinates $z^i$. This representation is much closer to the Fock representation as is clear from quantum mechanics where the basis states $|n_j\rangle$ are given by the functions $\langle z_i|n_j\rangle = z_i^n$. We shall leave the comparison between these two functional description for a future publication.

**Acknowledgments**

We would like to thank A. Ashtekar for discussions, R. Jackiw for drawing our attention to Refs. 3, 4 and J. Velhinho for comments. This work was in part supported by DGAPA-UNAM grant No. IN112401, by CONACyT grants J32754-E and 36581-E, NSF grant No. PHY-0010061, and US DOE grant DE-FG03-91ER40674. J.C. was supported by a UNAM (DGEP)-CONACyT Graduate Fellowship. H.Q. thanks UC-MEXUS for support.

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3 Recall that in the case of Minkowski spacetime and for flat embeddings, where $\Sigma$ is a Euclidean space, the quantum configuration space is the space of tempered distributions $\mathcal{S}^*$ on $\Sigma$. However, in order to define this space one uses the linear and Euclidean structure of $\Sigma$ and its generalization to curved manifolds is not trivial.
Let us consider in this section the example of a simple harmonic oscillator in $N$ dimensions. The configuration space is $C = \{q^i\}$, and the phase space $\Gamma = (q^i, p_i)$. The symplectic structure is given by

$$\Omega_{ab} = 2\nabla_a p_i \nabla_b q^i,$$

such that $\{q^i, p_j\} = \delta^i_j$. The standard complex structure $J$ compatible with the symplectic two form is

$$J^a_b = \left( \frac{\partial}{\partial p_i} \right)^a \nabla b q^i - \left( \frac{\partial}{\partial q^i} \right)^a \nabla b p_i.$$  \hfill (A1)

It is straightforward to see that the induced metric $\mu_{ab} : J^a_c \Omega_{cb}$ is given by

$$\mu_{ab} = \nabla_a q^b \nabla b q_i + \nabla_a \nabla b p_i.$$  \hfill (A2)

The complex structure then has the following action on the basis vectors on $\mathbb{T}T$, \hfill (A3)

$$J \cdot \left( \frac{\partial}{\partial q^i} \right) = \left( \frac{\partial}{\partial p_i} \right) \quad \text{and} \quad J \cdot \left( \frac{\partial}{\partial p_i} \right) = - \left( \frac{\partial}{\partial q^i} \right).$$

Let us now consider the observables. Now the vector indicated by $Y^a = (q^i, p_j)^a$ is given by,

$$Y^a = q^i \left( \frac{\partial}{\partial q^i} \right)^a + p_i \left( \frac{\partial}{\partial p_i} \right)^a$$

and the one-form $\lambda_a = (-\alpha_i, -\beta^j) \lambda_a$ is given by,

$$\lambda_a = -\alpha_i (\nabla_a q^i) - \beta^j (\nabla_a p_i)$$

such that

$$F_\lambda(Y) := -\lambda_a Y^a = \alpha_i q^i + \beta^j p_i.$$  \hfill (A4)

Recall that there is also a label vector given by $(-\beta, \alpha)^a$, that gives rise to particular configuration and momentum observables as follows

$$Q(\alpha_i) := F_{(-\alpha, 0)}(Y) = \Omega_{ab}(0, \alpha_i)^a(q^k, p_j)^b = \alpha_i q^i$$

and

$$P(\beta^j) := F_{(0, -\beta)}(Y) = \Omega_{ab}(0, -\beta^i, 0)^a(q^k, p_j)^b = \beta^j p_i$$

Let us suppose that we have found a representation of the basic observables as operators, namely we have $\hat{q}^i$ and $\hat{p}_i$ acting on a Hilbert space $\mathcal{H}$. The corresponding operator is given by $\hat{O}((-\beta, \alpha)) := \alpha_i \hat{q}^i + \beta^j \hat{p}_i$. Let us now construct the creation and annihilation operators for a general observable:

$$\mathcal{C}((-\beta, \alpha)) := \frac{1}{2\hbar} \left[ \hat{O}(J \cdot (-\beta, \alpha)) + i \hat{O}((-\beta, \alpha)) \right] = \frac{1}{2\hbar} \left[ (-\beta_i + i\alpha_i)(\hat{q}^i - i\hat{p}_i) \right]$$  \hfill (A5)

and for the annihilation operator we have,

$$\mathcal{A}((-\beta, \alpha)) := \frac{1}{2\hbar} \left[ \hat{O}(J \cdot (-\beta, \alpha)) - i \hat{O}((-\beta, \alpha)) \right] = \frac{1}{2\hbar} \left[ (-\beta_i - i\alpha_i)(\hat{q}^i + i\hat{p}_i) \right]$$

Let us note that if we define the operators,

$$\hat{a}^{\dagger} := \frac{1}{\sqrt{2\hbar}} (\hat{q}^i - i\hat{p}_i)$$ \hfill (A6)

and,

$$\hat{a} := \frac{1}{\sqrt{2\hbar}} (\hat{q}^i + i\hat{p}_i)$$ \hfill (A7)

and the complex coordinates $\zeta^i := \frac{1}{\sqrt{2\hbar}} (-\beta^i + i\alpha^i)$, then we have

$$\mathcal{C}((-\beta, \alpha)) = \zeta_i \hat{a}^{\dagger} \quad \text{and} \quad \mathcal{A}((-\beta, \alpha)) = \bar{\zeta}_i \hat{a}^{\dagger}$$ \hfill (A8)

Thus, we get the standard relations between the ordinary Schrödinger and the oscillator representation, making also contact between the notation we have used of defining the creation of a state labelled by a ‘label vector’ $\zeta$ and the ordinary creation and annihilation operators used elsewhere.
APPENDIX B: NON-TRIVIAL VACUA

In Sec. [IV A] we discussed the possibility of defining a Schrödinger representation in which the measure is the “homogeneous” one. As mentioned before, this representation does not exist from a rigorous viewpoint since the homogeneous measure is not well defined \[19\]. However, one can ignore this and pretend that this representation exists. We expect that in analogy with the harmonic oscillator, in this case the vacuum will have a Gaussian form.

However, there is no a-priori expression for it. The purpose of this appendix is to develop this reasoning, and construct then the non-trivial vacua associated to the Gaussian measures. We know from the general discussion in Sec. [IV A] that the “momentum operator” associated to an homogeneous measure is represented as follows (\(\hbar = 1\)):

\[
\hat{\pi}[g] = -i \int d^3x \, g(x) \frac{\delta}{\delta \varphi(x)}.
\]  

(B1)

Now, applying the equation for the vacuum \(\Psi_0\), namely \(A(\zeta) \cdot \Psi_0 = 0\) for all \(\zeta \in \Gamma\), we get from (5.5) that (with \(\hbar = 1\))

\[
A(-g, f) \cdot \Psi_0 = \frac{1}{2} \int_\Sigma \left( \varphi [Dg - Cf - if] + [iAg - g - iBf] \frac{\delta}{\delta \varphi} \right) \Psi_0 = 0.
\]  

(B2)

Let \(\Lambda\) be such that \(\delta \Psi_0[\varphi]/\delta \varphi = \Lambda \Psi_0[\varphi]\). Then,

\[
\int_\Sigma \left( \varphi [Dg - Cf - if] + \Lambda [iAg - g - iBf] \right) \Psi_0 = 0
\]

(B3)

for all \((-g, f) \in \Gamma\). Given that \(g\) and \(f\) are independent, the last equation should be valid for all vectors of the type \((0, f) \in \Gamma\). Thus, using the first and last relation in (4.14) we have that

\[
\int_\Sigma (f (iB + [i - A]) \Psi_0 = 0; \forall f
\]

(B4)

which implies that \((1 + iA)\varphi + BA = 0\), then \(\Lambda = -B^{-1} \varphi - iB^{-1} A\varphi = -(1 - iC)B^{-1} \varphi\) (where we have used that \(B^{-1} A = -CB^{-1}\)). We can now verify that, for all \(g\),

\[
\int_\Sigma \left( \varphi Dg + \Lambda [iAg - g] \right) \Psi_0 = \int_\Sigma g \left( D\varphi - iC\Lambda - \Lambda \right) \Psi_0
\]

(B5)

vanishes after substituting the expression for \(\Lambda\) and using the conditions satisfied by the operators \(A, B, C, D\). Thus, we can conclude that the condition in the vacuum reads,

\[
\frac{\delta \Psi_0[\varphi]}{\delta \varphi} = -[(1 - iC)B^{-1} \varphi] \Psi_0[\varphi] =: -(Q \cdot \varphi) \Psi_0[\varphi],
\]

(B6)

where we have defined the operator \(Q := (1 - iC)B^{-1}\). We make then the ansatz,

\[
\Psi_0[\varphi] = e^{\alpha \int_\Sigma \varphi Q \cdot \varphi}.
\]

Let us now show that this state indeed satisfies (B6). Let \(\{\varphi_\lambda\}\) be a one parameter family of field configurations and \(\delta \varphi := d\varphi_\lambda/d\lambda|_{\lambda=0}\), then,

\[
\frac{d\Psi_0}{d\lambda} = \alpha \int_\Sigma \left[ \frac{d\varphi_\lambda}{d\lambda} (Q \cdot \varphi_\lambda) + \varphi_\lambda \left( Q \cdot \frac{d\varphi_\lambda}{d\lambda} \right) \right] \Psi_0 = \alpha \int_\Sigma [\hat{\varphi}_\lambda Q \cdot \varphi_\lambda + \varphi_\lambda Q \cdot \varphi_\lambda] \Psi_0
\]

(B7)

where \(\hat{\varphi}_\lambda := d\varphi_\lambda/d\lambda\). Let us consider the term of the form \(\int g \varphi g'\), for all \(g\) and \(g'\) in \(C_0^\infty(\Sigma)\). Since \(B\) is symmetric, \(B^{-1}\) will also be, and then \(\int g \varphi g' = \int g' B^{-1} g - i \int g' C B^{-1} g'\), but since \(\int g' C B^{-1} g' = -\int Ag (B^{-1} g') = -\int g' B^{-1} Ag\), using the identity \(B^{-1} A = -CB^{-1}\) we have that \(\int g' C B^{-1} g' = \int g' CB^{-1} g\). Therefore, \(Q\) is symmetric. Hence, we can conclude that,

\[
\frac{d\Psi_0}{d\lambda} \bigg|_{\lambda=0} = \int_\Sigma [\hat{\varphi}_\lambda (2\alpha Q \cdot \varphi_\lambda)] \Psi_0|_{\lambda=0} = \int_\Sigma \delta \varphi \left[ \frac{\delta \Psi_0[\varphi]}{\delta \varphi} \right],
\]

(B8)
which implies that $\delta \Psi_0[\phi]/\delta \phi = 2\alpha (Q \cdot \phi) \Psi_0[\phi]$. Therefore, $\alpha = -1/2$ and the vacuum, in the “homogeneous” Schrödinger representation, is given by the functional,

$$\Psi_0[\phi] = e^{-\frac{1}{2} \int_{\Sigma} \phi (B^{-1} \cdot \nabla B^{-1}) \phi}.$$  

(B10)

Thus, if we were to absorb the vacuum into the measure, we would have $d\mu = D\phi \Psi_0 \Psi_0 = D\phi \int_{\Sigma} e^{\phi (B^{-1} \cdot \nabla B^{-1}) \phi}$ which is precisely the Gaussian measure given by (4.20).

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