

Schrödinger representation for a scalar field on curved spacetime

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It is generally known that linear (free) field theories are one of the few quantum field theories that are exactly soluble. In the Schrödinger functional description of a scalar field on flat Minkowski spacetime and for flat embeddings, it is known that the usual Fock representation is described by a Gaussian measure. In this paper, arbitrary globally hyperbolic spacetimes and embeddings of the Cauchy surface are considered. The classical structures relevant for quantization are used for constructing the Schrödinger representation in the general case. It is shown that, in this case, the measure is also Gaussian. Possible implications for the program of canonical quantization of midisuperspace models are pointed out.

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I. INTRODUCTION

The quantum theory of a free real scalar field is probably the simplest field theory system. Indeed, it is studied in the first chapters of most field theory textbooks [1]. 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. However, from the perspective of “canonical quantization,” where one starts from a classical Poisson algebra and performs a quantization of the system, this procedure is not always transparent. These issues have been addressed by Wald who, motivated by the study of quantum fields on curved spacetimes, deals with the process of quantization, starting from a classical algebra of observables and constructing representations of them on Hilbert spaces [2]. Furthermore, Wald develops the quantum theory of a scalar field and extends the formalism to an arbitrary globally hyperbolic 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 hand, the usual presentation of elementary quantum mechanics pays a lot of attention to the Schrödinger representation, where quantum states are represented by functions on configuration space. Thus, the construction of the functional Schrödinger representation for fields seems to be a natural step in this direction. It is therefore unsettling that a complete and detailed treatment for curved spacetimes does not seem to be available in the literature. The purpose of this paper is to fill this gap. The Schrödinger representation for fields on *Minkowski* spacetime, where an inertial

slicing of the spacetime is normally introduced, has been previously studied (for reviews, see [3]). This functional viewpoint, though 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 quantum field theory.¹

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 [4]). This is especially true since some symmetry-reduced gravitational system 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 [5] and Gowdy cosmologies [6,7]. The Schrödinger picture is then, 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.

In this regard, there seems to be apparent tension in the construction of the Schrödinger representation for a scalar field. On the one hand, if one follows a systematic approach to quantization, as outlined, for instance, in [8,9], one can, without difficulties, arrive at the “ordinary” representation of the elementary quantum operators [3,4,10], where the quantum measure is “homogeneous.” However, we know from the more rigorous treatments of the subject [11–13] that a consistent quantization should involve a nonhomogeneous, Gaussian measure, and therefore a nonstandard representation of the (momentum) operators. This seems to indicate that one needs additional “dynamical” input within the algebraic quantization procedure [8,9].

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The purpose of this paper is to systematically construct the functional quantum theory and extend the rigorous formalism of [11,12] to arbitrary embeddings of the Cauchy surface and to arbitrary curved spacetimes, in the spirit of [2]. The emphasis we shall place regarding the relevant structures will allow us to achieve this goal. The generalization that we will construct in this paper will be at two levels. To be specific, we first deal with the existing ambiguity in the quantization of a scalar field, already recognized in the Fock quantization [2]. Furthermore, the infinite freedom in the choice of embedding of the Cauchy surface is considered. We find that the measure is always Gaussian in an appropriate sense and that it can be written in a simple way. Even when straightforward, these results have not, to the best of our knowledge, appeared elsewhere. As an offspring, they provide the required language for the systematic treatment of symmetry-reduced models within canonical quantum gravity [5–7], and provide an elegant solution to the apparent tension mentioned above.

The structure of the paper is as follows. In Sec. II, we recall basic notions from the classical formulation of a scalar field. A discussion of the Schrödinger representation and construction of the functional description, unitarily equivalent to a given Fock representation, is the subject of Sec. III. This is the main section of the paper. We end with a discussion in Sec. IV.

In order to make this work accessible not only to specialized researchers in theoretical physics, we have intentionally avoided going into detail 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.

II. CLASSICAL PRELIMINARIES

In this section, we recall the classical theory of a real, linear Klein-Gordon field ϕ with mass m propagating on a four-dimensional, globally hyperbolic spacetime $({}^4M, g_{ab})$. As is well known, global hyperbolicity implies that 4M has topology $\mathbf{R} \times \Sigma$, and can be foliated by a one-parameter family of smooth Cauchy surfaces diffeomorphic to Σ . Hence, we can perform a 3+1 decomposition of the spacetime of the form $\mathbf{R} \times \Sigma$ and consider arbitrary embeddings of the surface Σ into 4M .

This section has two parts. In the first one, we recall the canonical treatment of the scalar field, together with the observables that are relevant for quantization. In the second part, we introduce a classical construct that is needed for quantization, namely a complex structure on phase space.

A. Canonical phase space and observables

The phase space of the theory can be alternatively described by the space Γ of Cauchy data (in the canonical approach), that is, $\{(\varphi, \pi) | \varphi: \Sigma \rightarrow \mathbf{R}, \pi: \Sigma \rightarrow \mathbf{R}; \varphi, \pi$

$\in C_0^\infty(\Sigma)\}$,² or by the space V of smooth solutions to the Klein-Gordon equation which arises from initial data on Γ (in the covariant formalism) [2]. Note that, for each embedding $T_t: \Sigma \rightarrow {}^4M$, there exists an isomorphism \mathcal{I}_t between Γ and V . The key observation is that there is a one-to-one correspondence between a pair of initial data of compact support on Σ , and solutions to the Klein-Gordon equation on 4M . That is to say, given an embedding T_{t_0} of Σ as a Cauchy surface $T_{t_0}(\Sigma)$ in 4M , the (natural) isomorphism $\mathcal{I}_{t_0}: \Gamma \rightarrow V$ is obtained by taking a point in Γ and evolving from the Cauchy surface $T_{t_0}(\Sigma)$ to get a solution of $(g^{ab}\nabla_a\nabla_b - m^2)\phi = 0$. That is, the specification of a point in Γ is the appropriate initial data for determining a solution to the equation of motion. The inverse map, $\mathcal{I}_{t_0}^{-1}: V \rightarrow \Gamma$, takes a point $\phi \in V$ and finds the Cauchy data induced on Σ by virtue of the embedding $T_{t_0}: \varphi = T_{t_0}^*\phi$ and $\pi = T_{t_0}^*(\sqrt{h}\mathcal{L}_n\phi)$, where \mathcal{L}_n is the Lie derivative along the normal to the Cauchy surface $T_{t_0}(\Sigma)$ and h is the determinant of the induced metric on such a surface. Note that the phase space Γ is of the form $T^*\mathcal{C}$, where the classical configuration space \mathcal{C} is comprised of the set of smooth real functions of compact support on Σ .

Since the phase space Γ is a linear space, there is a particular simple choice for the set of fundamental observables. We can take a global chart on Γ and we can choose the set of fundamental observables to be the vector space generated by linear functions on Γ . More precisely, classical observables for the space Γ can be constructed directly by giving smearing functions on Σ . We can define linear functions on Γ as follows: given a vector Y^α in Γ of the form $Y^\alpha = (\varphi, \pi)^\alpha$ (note that due to the linear nature of Γ , Y^α also represents a vector in $T\Gamma$) and a pair $\lambda_\alpha = (-f, -g)_\alpha$, where f is a scalar density and g a scalar, we define the action of λ on Y as

$$F_\lambda(Y) = -\lambda_\alpha Y^\alpha := \int_\Sigma (f\varphi + g\pi) d^3x. \quad (2.1)$$

Now, since in the phase space Γ the symplectic structure Ω takes the following form, when acting on vectors (φ_1, π_1) and (φ_2, π_2) ,

$$\Omega([\varphi_1, \pi_1], [\varphi_2, \pi_2]) = \int_\Sigma (\pi_1\varphi_2 - \pi_2\varphi_1) d^3x, \quad (2.2)$$

then we can write the linear function (2.1) 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 one-form on phase space can also be

²The class of functions comprised by Schwartz space is most commonly chosen for quantum field theory in Minkowski spacetime. However, the notion of Schwartz space is not extendible in any obvious way to more general manifolds [2,14]. Hence, we shall define Γ to consist of initial data which are smooth and of compact support on Σ .

seen as the vector $(-g, f)^\beta$. Note that the role of the smearing functions is interchanged in the passing from a one-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 on specific choices for the label λ . 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

$$\varphi[f] := \int_{\Sigma} d^3x f \varphi. \quad (2.3)$$

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

$$\pi[g] := \int_{\Sigma} d^3x g \pi. \quad (2.4)$$

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 Σ , 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 confusion, we shall make the distinction between *label vectors* $(-g, f)^\alpha$ and *coordinate vectors* $(\varphi, \pi)^\alpha$.

It is important to emphasize that the symplectic structure provides the space of classical observables with an algebraic structure via the Poisson brackets (PB). If we are now given another label ν , such that $G_\nu(Y) = \nu_\alpha Y^\alpha$, we can compute the Poisson brackets

$$\{F_\lambda, G_\nu\} = \Omega^{\alpha\beta} \nabla_\alpha F_\lambda(Y) \nabla_\beta G_\nu(Y) = \Omega^{\alpha\beta} \lambda_\alpha \nu_\beta. \quad (2.5)$$

Since the two-form is nondegenerate, we can rewrite it as $\{F_\lambda, G_\nu\} = -\Omega_{\alpha\beta} \lambda^\alpha \nu^\beta$. Thus,

$$\{\Omega(\lambda, Y), \Omega(\nu, Y)\} = -\Omega(\lambda, \nu). \quad (2.6)$$

B. Complex structure

Now, in order to provide the canonical approach with the mathematical structure that encodes the inherent ambiguity in QFT, and exactly in the same sense as it is done for the Fock quantization, we have to introduce at the classical level a complex structure on the canonical phase space Γ , compatible with the symplectic structure (2.2). Recall that in the Fock picture, which is naturally constructed from the covariant phase space V , the complex structure is compatible with the symplectic form defined on that space (a complex structure is a linear mapping such that $J^2 = -1$). Now, for the canonical phase space, given an embedding $T_{t_0}: \Sigma \rightarrow {}^4M$ and a complex structure on V , there is one complex structure on Γ induced by virtue of the symplectic map \mathcal{I}_{t_0} . On the symplectic vector space (Γ, Ω) with coordinates (φ, π) , the most general form of the complex structure J is given by

$$-J_\Gamma(\varphi, \pi) = (A\varphi + B\pi, C\pi + D\varphi), \quad (2.7)$$

where A, B, C , and D are linear operators satisfying the following relations [15]:

$$\begin{aligned} A^2 + BD &= -\mathbf{1}, & C^2 + DB &= -\mathbf{1}, \\ AB + BC &= 0, & DA + CD &= 0. \end{aligned} \quad (2.8)$$

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

$$\begin{aligned} \mu_\Gamma((\varphi_1, \pi_1), (\varphi_2, \pi_2)) &= \int_{\Sigma} d^3x (\pi_1 B \pi_2 + \pi_1 A \varphi_2 - \varphi_1 D \varphi_2 \\ &\quad - \varphi_1 C \pi_2), \end{aligned} \quad (2.9)$$

for all pairs (φ_1, π_1) and (φ_2, π_2) . As μ_Γ is symmetric, then the linear operators should also satisfy [15]

$$\begin{aligned} \int_{\Sigma} f B f' &= \int_{\Sigma} f' B f, & \int_{\Sigma} g D g' &= \int_{\Sigma} g' D g, \\ \int_{\Sigma} f A g &= - \int_{\Sigma} g C f, \end{aligned} \quad (2.10)$$

where $g, g' \in C_0^\infty(\Sigma)$ are scalars and $f, f' \in C_0^\infty(\Sigma)$ are scalar densities of weight 1.

As mentioned before, given an embedding T_{t_0} of Σ there is a one-to-one correspondence between complex structures on V and Γ . That is, if we have a particular isomorphism \mathcal{I}_{t_0} , the complex structure induced on Γ by J_V , a particular complex structure on the covariant phase space, is given by $J_\Gamma = \mathcal{I}_{t_0}^{-1} J_V \mathcal{I}_{t_0}$. This relation and the general form (2.7) implies that

$$\begin{aligned} A\varphi + B\pi &= -T_{t_0}^*[J_V \phi], \\ C\pi + D\varphi &= -T_{t_0}^*[\sqrt{\hbar} \mathcal{E}_n(J_V \phi)], \end{aligned} \quad (2.11)$$

where $\phi = \mathcal{I}_{t_0}(\varphi, \pi)$ [i.e., ϕ is the solution to the Klein-Gordon equation which arises from the Cauchy data pair (φ, π)]. Thus, the particular realization of the operators A, B, C , and D will be different for different embeddings T_t of Σ .

III. SCHRÖDINGER REPRESENTATION

In this section, we turn our attention to the Schrödinger representation. In contrast with the Fock case, which is most naturally stated and constructed in a covariant framework [2], this construct relies heavily on a Cauchy surface Σ , since its most naive interpretation is in terms of a “wave functional at time t .”

Let us begin by looking at the classical observables that are to be quantized, and in terms of which the canonical commutation relations (CCR) are expressed. Since the vector space of elementary classical variables is $\mathcal{S} = \text{Span}\{1, \varphi[f], \pi[g]\}$ and there is an abstract operator \hat{F} in the free associative algebra generated by \mathcal{S} associated with each element F in \mathcal{S} , then we have that the basic quantum operators are $\hat{\varphi}[f]$ and $\hat{\pi}[g]$. The canonical commutation relations arise by imposing the Dirac quantization condition on the basic quantum operators, thus from Eqs. (2.3), (2.4), and (2.6), the CCR read $[\hat{\varphi}[f], \hat{\pi}[g]] = i\hbar \int d^3x f g \hat{\mathbf{1}}$ (for a

general discussion and details about the set \mathcal{S} and the steps for passage to quantum theory in the canonical framework, see [8]).

Now, the Schrödinger representation, at least in an intuitive level, is to consider “wave functions” as function(al)s of φ . More precisely, the Schrödinger picture consists in representing the abstract operators $\hat{\varphi}[f]$ and $\hat{\pi}[g]$ as operators in $\mathcal{H}_s := L^2(\bar{\mathcal{C}}, d\mu)$, where a state would be represented by a function(al) $\Psi[\varphi]: \bar{\mathcal{C}} \rightarrow \mathbf{C}$, with the appropriate “reality conditions,” which in our case means that these operators should be Hermitian.

As a first trial, inspired and tempted by the names “configuration” and “momentum,” one can try to represent the corresponding operators as is done in ordinary quantum mechanics, namely, by multiplication and derivation, respectively. However, one must be careful since, in contrast to ordinary quantum mechanics, the configuration space of the theory is now infinite dimensional and Lebesgue-type measures are no longer available. (The theory of measures on infinite-dimensional vector spaces has some subtleties, among which is the fact that well-defined measures should be *probability* measures [14,16]. A uniform measure would not have such a property.) As a consequence of the intimate relation between measure and operator representation, and in order to reflect the nonexistence of a homogeneous measure in a consistent way, we have to modify a bit the simplest extension (suggested by ordinary quantum mechanics) and represent the basic operators, when acting on functionals $\Psi[\varphi]$, as follows:

$$(\hat{\varphi}[f] \cdot \Psi)[\varphi] := \varphi[f] \Psi[\varphi] \quad (3.1)$$

and

$$\begin{aligned} (\hat{\pi}[g] \cdot \Psi)[\varphi] := & -i\hbar \int_{\Sigma} d^3x g(x) \frac{\delta \Psi}{\delta \varphi(x)} \\ & + \text{multiplicative term,} \end{aligned} \quad (3.2)$$

where the second term in Eq. (3.2), depending only on configuration variable, is precisely there to render the operator self-adjoint when the measure is different from the “homogeneous” measure, and depends on the details of the measure. The first thing to note is that the representation is not fixed “canonically.” That is, we need to know the measure in order to represent the momentum observable. This is in sharp contrast with the strategy followed in the algebraic method [8], where one first represents the operators and later looks for a measure that renders the operators Hermitian. It seems that, even for the simplest field theory system, one needs to modify the strategy slightly.

Observe that we have already encountered two new actors in the play. The first is the *quantum configuration space* $\bar{\mathcal{C}}$, and the second one is the measure μ thereon. Thus, one will need to specify these objects in the construction of the theory. To do this, we will carry out a two-step process. First we need to find the measure $d\mu$ on the quantum configura-

tion space in order to get the Hilbert space \mathcal{H}_s , and second we need to find the multiplicative term of the basic operator (3.2).

The strategy that seems natural to determine the measure and the multiplicative term is to suppose that we possess a Fock representation (it does not matter which particular one, since the results will be general enough). This representation must have a unitarily equivalent counterpart in the Schrödinger picture, and therefore fixes the measure and the multiplicative operator in the functional framework. That is, given a Fock representation, we want to find the Schrödinger representation that is equivalent to that one. In the remainder of this section, we will dedicate Sec. III A to formulating this equivalence in a precise way and Sec. III B to completing the Schrödinger representation.

A. Quantum algebra and states

We shall start by assuming the existence of a consistent Fock representation of the CCR. The question we want to address now is how to formulate equivalence between the two different representations for the theory. The most natural way to define this notion is through the algebraic formulation of QFT (see [17,12], and [2] 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 (i) a C^* algebra \mathcal{A} of observables, and (ii) states $\omega: \mathcal{A} \rightarrow \mathbf{C}$, which are positive linear functionals [$\omega(A^*A) \geq 0 \forall A \in \mathcal{A}$] such that $\omega(1) = 1$. The value of the state ω acting on the observable A can be interpreted as the expectation value of the operator A on the state ω , 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 (2.1), labeled by a phase-space vector λ^α . These generators satisfy the Weyl relations,

$$W(\lambda)^* = W(-\lambda),$$

$$W(\lambda_1)W(\lambda_2) = e^{(i/2)\Omega(\lambda_1, \lambda_2)} W(\lambda_1 + \lambda_2). \quad (3.3)$$

The CCR [$\hat{\Omega}(\lambda, \cdot), \hat{\Omega}(\nu, \cdot) = -i\hbar \Omega(\lambda, \nu) \hat{1}$] now get replaced by the quantum Weyl relations where now the operators $\hat{W}(\lambda)$ belong to the (abstract) algebra \mathcal{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 Gelfand, Neumark, Segal (GNS) construction that can be stated as the following theorem [2].

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

$$\omega(A) = \langle \Psi_0, \pi(A) \Psi_0 \rangle_{\mathcal{H}}. \quad (3.4)$$

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 know exactly how to construct a Fock representation from the symplectic vector space (V, Ω_V) endowed with a complex structure J [2]. The infinite-dimensional freedom in the choice of representation of the CCR relies on the choice of admissible J , which gives rise to the one-particle Hilbert space³ \mathcal{H}_0 . Thereafter, the construction is completely natural and there are no further choices to be made: We take the Hilbert space of the QFT to be $\mathcal{F}_s(\mathcal{H}_0)$. The fundamental observables $\hat{\Omega}(\phi, \cdot)$ on $\mathcal{F}_s(\mathcal{H}_0)$ are then defined by $\hat{\Omega}(\phi, \cdot) = iA(\overline{K\phi}) - iC(K\phi)$, where C and A are, respectively, the creation and annihilation operators, and K is the restriction to V of the orthogonal projection map $\underline{K}: V_\mu^C \rightarrow \mathcal{H}_0$ in the inner product $\mu(\phi_1, \phi_2) = -i\Omega(\phi_1, \phi_2)$. Hence, if we suppose that we have a complex structure on V (i.e., a Fock representation), we can now compute the expectation value of the Weyl operators on the Fock vacuum and thus obtain a positive linear functional ω_{Fock} on the algebra \mathcal{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 ω_{Fock} . Our job now is to complete the Schrödinger construction such that the expectation values 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 . By hypothesis, we have a triplet $(\mathcal{F}_s(\mathcal{H}_0), R_{\text{Fock}}, \Omega_{\mathcal{F}_s(\mathcal{H}_0)})$, where (i) $\mathcal{F}_s(\mathcal{H}_0)$ is the symmetric Fock space specified by some complex structure, (ii) R_{Fock} is a map from the Weyl algebra to the collection of all bounded linear maps on $\mathcal{F}_s(\mathcal{H}_0)$ [R_{Fock} sends the Weyl generator $\hat{W}(\phi)$, labeled by ϕ , to the operator $\exp[i\hat{\Omega}(\phi, \cdot)] \in L(\mathcal{F}_s(\mathcal{H}_0))$, and is extendable to the whole algebra by linearity and continuity], and (iii) $\Omega_{\mathcal{F}_s(\mathcal{H}_0)}$ is the vacuum state of the theory. Thus, by virtue of the GNS construction, the value of the state ω_{Fock} acting on the Weyl generators $\hat{W}(\phi)$ is interpreted as the expectation value of the corresponding operators $R_{\text{Fock}}(\hat{W}(\phi))$ on the vacuum state $\Omega_{\mathcal{F}}$ [from now on we replace $\mathcal{F}_s(\mathcal{H}_0)$ by \mathcal{F}],

$$\omega_{\text{Fock}}(\hat{W}(\phi)) = \langle \Omega_{\mathcal{F}}, R_{\text{Fock}}(\hat{W}(\phi)) \Omega_{\mathcal{F}} \rangle_{\mathcal{F}}. \quad (3.5)$$

Now, since $R_{\text{Fock}}(\hat{W}(\phi)) = \exp[i\hat{\Omega}(\phi, \cdot)] = \exp(C(K\phi)$

$-A(\overline{K\phi}))$, we can rewrite, by using the Baker-Campbell-Hausdorff relation, the corresponding operator to the Weyl generator as follows:

$$R_{\text{Fock}}(\hat{W}(\phi)) = \exp(C(K\phi)) \exp(-A(\overline{K\phi})) \times \exp(-\frac{1}{2}[A(\overline{K\phi}), C(K\phi)]). \quad (3.6)$$

But the commutator $[A(\overline{K\phi}), C(K\phi)]$ is equal to $(\overline{K\phi})_A(K\phi)^A \hat{1}$. Thus, since

$$\begin{aligned} (\overline{K\phi_1})_A(K\phi_2)^A &= (K\phi_1, K\phi_2)_{\mathcal{H}_0} \\ &= \frac{1}{2} \mu(\phi_1, \phi_2) - \frac{i}{2} \Omega(\phi_1, \phi_2), \end{aligned} \quad (3.7)$$

then $(\overline{K\phi})_A(K\phi)^A = \frac{1}{2} \mu(\phi, \phi)$. Therefore, the vacuum expectation value of $R_{\text{Fock}}(\hat{W}(\phi))$ is given by

$$\begin{aligned} \langle R_{\text{Fock}}(\hat{W}(\phi)) \rangle_{\text{vac}} &= \langle \Omega_{\mathcal{F}}, \exp(C(K\phi)) \\ &\quad \times \exp(-A(\overline{K\phi})) \Omega_{\mathcal{F}} \rangle_{\mathcal{F}} \\ &\quad \times \exp(-\frac{1}{4} \mu(\phi, \phi)). \end{aligned} \quad (3.8)$$

Because $\langle \Omega_{\mathcal{F}}, \Psi \rangle_{\mathcal{F}} = 0$ for all $\Psi \in \mathcal{F}$ such that $\Psi = (0, \phi^{A_1}, \phi^{(A_1 A_2)}, \dots, \phi^{(A_1 \dots A_n)}, \dots)$, then $\langle \Omega_{\mathcal{F}}, \exp(C(K\phi)) \exp(-A(\overline{K\phi})) \Omega_{\mathcal{F}} \rangle_{\mathcal{F}} = \langle \Omega_{\mathcal{F}}, \Omega_{\mathcal{F}} \rangle_{\mathcal{F}}$. Hence, if the vacuum state is normalized, substituting $\langle R_{\text{Fock}}(\hat{W}(\phi)) \rangle_{\text{vac}}$ in Eq. (3.5) we obtain that the value of the state ω_{Fock} acting on the Weyl generators $\hat{W}(\lambda)$ is given by the following expression:

$$\omega_{\text{Fock}}(\hat{W}(\lambda)) = e^{-(1/4)\mu(\lambda, \lambda)}, \quad (3.9)$$

where, thanks to the symplectic map \mathcal{I}_t , we were able to put λ as a label vector for both covariant and canonical approaches. Note that the GNS construction is precisely the technology that allows us to invert the process. That is, from the point of view of the algebraic approach, the choice of a complex structure J defines the Fock representation via the GNS construction based upon a state ω_{Fock} , which is defined on the basic generators of the Weyl algebra by Eq. (3.9).

B. Functional representation

The next step is to complete the Schrödinger representation. That is, find the measure $d\mu$ and the multiplicative term in Eq. (3.2) that corresponds to the given Fock representation.

In order to specify the measure $d\mu$ that defines the Hilbert space, it suffices to consider configuration observables. Now, we know how to represent these observables *independently* of the measure since they are represented as multiplication operators as given by Eq. (3.1). The Weyl observable $\hat{W}(\lambda)$ corresponding to $(0, f)^\alpha$ in the Schrödinger picture has the form

$$R_{\text{sch}}(\hat{W}(\lambda)) = e^{i\hat{\phi}[f]}. \quad (3.10)$$

Now, Eq. (3.9) tells us that the state ω_{sch} should be such that

³It is worth pointing out that from the infinite possible J there are physically inequivalent representations [2], a clear indication that the Stone-von Neumann theorem does not generalize to field theories.

$$\begin{aligned}\omega_{\text{sch}}(\hat{W}(\lambda)) &= \exp\left[-\frac{1}{4}\mu(\lambda, \lambda)\right] \\ &= \exp\left[-\frac{1}{4}\int_{\Sigma} d^3x f B f\right],\end{aligned}\quad (3.11)$$

where we have used Eq. (2.9) in the last step. On the other hand, the left hand side of Eq. (3.9) is the vacuum expectation value of the $\hat{W}(\lambda)$ operator. That is,

$$\begin{aligned}\omega_{\text{sch}}(\hat{W}(\lambda)) &= \int_{\bar{\mathcal{C}}} d\mu \bar{\Psi}_0 [R_{\text{sch}}(\hat{W}(\lambda)) \cdot \Psi_0] \\ &= \int_{\bar{\mathcal{C}}} d\mu e^{i\int_{\Sigma} d^3x f \varphi}.\end{aligned}\quad (3.12)$$

Let us now compare Eqs. (3.11) and (3.12),

$$\int_{\bar{\mathcal{C}}} d\mu e^{i\int_{\Sigma} d^3x f \varphi} = \exp\left[-\frac{1}{4}\int_{\Sigma} d^3x f B f\right].\quad (3.13)$$

At this point, we take a brief *detour* in order to understand the meaning of Eq. (3.13). Since in the case of infinite-dimensional vector spaces \mathcal{V} , the *Fourier transform* of the measure $\tilde{\mu}$ is defined as

$$\chi_{\tilde{\mu}}(f) := \int_{\mathcal{V}} d\tilde{\mu} e^{if(\varphi)},$$

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

$$\chi_{\tilde{\mu}}(f) = \exp\left(-\frac{1}{2}\langle f, Of \rangle_{\mathcal{V}}\right),\quad (3.14)$$

where $\langle \cdot, \cdot \rangle_{\mathcal{V}}$ is the Hermitian inner product on \mathcal{V} . We can, of course, ask what the measure $\tilde{\mu}$ looks like. The answer is that, schematically, it has the form

$$d\tilde{\mu} = \exp\left(-\frac{1}{2}\langle \varphi, O^{-1}\varphi \rangle_{\mathcal{V}}\right) \mathcal{D}\varphi,\quad (3.15)$$

where $\mathcal{D}\varphi$ represents the fictitious ‘‘Lebesgue-like’’ measure on \mathcal{V} . The expression (3.15) should be taken with a grain of salt since it is not completely well defined [whereas Eq. (3.14) is]. It is nevertheless useful for understanding where the denomination of Gaussian comes from. The term $-\frac{1}{2}\langle \varphi, O^{-1}\varphi \rangle_{\mathcal{V}}$ is (finite and) negative definite, and gives to $\tilde{\mu}$ its Gaussian character.

Thus, returning to our particular case, we note from Eqs. (3.14) and (3.15) that Eq. (3.13) tells us that the measure $d\mu$ is Gaussian and that it corresponds heuristically to a measure of the form

$$d\mu = e^{-\int_{\Sigma} \varphi B^{-1} \varphi} \mathcal{D}\varphi.\quad (3.16)$$

This is the desired measure. However, we still need to find the ‘‘multiplicative term’’ in the representation of the momentum operator (3.2). For that, we will need the full Weyl algebra and Eq. (3.9). Let us denote by K the Hilbert space obtained by completing \mathcal{C} with respect to the fiducial inner product $(g, f) := \int_{\Sigma} g f$ [15]. We have to compute $\langle R_{\text{sch}}(\hat{W}(g, f)) \rangle_{\text{vac}} = \langle \Psi_0, \exp(i\hat{\varphi}[f] - i\hat{\pi}[g]) \Psi_0 \rangle$, so let us note that we need to use the Baker-Campbell-Hausdorff relation to separate the operators; i.e.,

$$\begin{aligned}\exp(i\hat{\varphi}[f] - i\hat{\pi}[g]) &= \exp(i\hat{\varphi}[f]) \exp(-i\hat{\pi}[g]) \\ &\quad \times \exp(-\frac{1}{2}[i\hat{\varphi}[f], -i\hat{\pi}[g]]).\end{aligned}\quad (3.17)$$

Given that $[\hat{\varphi}[f], \hat{\pi}[g]] = i\int_{\Sigma} f g \hat{1}$ ($\hbar = 1$), then substituting Eq. (3.17) in Eq. (3.4) and using Eq. (3.9) we have that

$$\begin{aligned}e^{-(1/4)\mu_{\Gamma}((g, f), (g, f))} &= \exp\left(-\frac{i}{2}\int_{\Sigma} f g\right) \langle \Psi_0, \exp(i\hat{\varphi}[f]) \\ &\quad \times \exp(-i\hat{\pi}[g]) \Psi_0 \rangle,\end{aligned}\quad (3.18)$$

since $\exp(-i/2\int_{\Sigma} f g \hat{1}) \Psi_0 = \exp(-i/2\int_{\Sigma} f g) \Psi_0$ and $\exp(-i/2\int_{\Sigma} f g)$ does not depend on φ .

Now,

$$\exp(-i\hat{\pi}[g]) \Psi_0 = \exp(-i\hat{M} + \hat{d}) \Psi_0,\quad (3.19)$$

with

$$\begin{aligned}-i\hat{M} \cdot \Psi &= \left(\int_{\Sigma} \varphi \hat{m} g\right) \Psi = -iM \Psi, \\ \hat{d} \cdot \Psi &= -\int_{\Sigma} g \frac{\delta \Psi}{\delta \varphi}.\end{aligned}\quad (3.20)$$

Given that $[-i\hat{M}, \hat{d}] \cdot \Psi = -i[\int_{\Sigma} g (\delta M / \delta \varphi)] \Psi$, then using the Baker-Campbell-Hausdorff relation, we can write the right-hand side (RHS) of Eq. (3.19) as $\exp((i/2)\int_{\Sigma} g (\delta M / \delta \varphi)) \exp(-i\hat{M}) \exp(\hat{d}) \Psi_0$, since M is linear in φ , and therefore $\delta M / \delta \varphi$ does not depend on φ . On the other hand, $\exp(\hat{d}) \Psi_0 = \Psi_0$ (since Ψ_0 is constant) and $\exp(-i\hat{M}) \Psi_0 = \exp(-iM) \Psi_0$. Thus, Eq. (3.19) is

$$\exp(-i\hat{\pi}[g]) \Psi_0 = \exp\left(\frac{i}{2}\int_{\Sigma} g \frac{\delta M}{\delta \varphi}\right) \exp(-iM) \Psi_0.\quad (3.21)$$

Substituting this last expression in Eq. (3.18), we have that

$$\begin{aligned}e^{-(1/4)\mu_{\Gamma}((g, f), (g, f))} &= e^{-(i/2)\int_{\Sigma} f g} e^{(i/2)\int_{\Sigma} g (\delta M / \delta \varphi)} \\ &\quad \times \int_{\bar{\mathcal{C}}} d\mu e^{i\int_{\Sigma} f \varphi} e^{-iM}.\end{aligned}\quad (3.22)$$

Using Eqs. (2.9) and (3.20), we have that Eq. (3.22) is

$$\begin{aligned}
 e^{-(1/4)\int_{\Sigma}(fBf+fAg-gDg-gCf)} &= e^{-(i/2)\int_{\Sigma}fg} e^{-(1/2)\int_{\Sigma}g\hat{m}g} \\
 &\times \int_{\bar{\mathcal{C}}} d\mu e^{i\int_{\Sigma}(f-i\hat{m}g)\varphi}.
 \end{aligned} \tag{3.23}$$

From the last relation in Eq. (2.10), and using the fact that the integral on $\bar{\mathcal{C}}$ is the Fourier transform with $f \mapsto (f - i\hat{m}g)$ of the measure (3.16), we get

$$\begin{aligned}
 e^{-(1/4)\int_{\Sigma}(fBf-gDg+2fAg)} &= e^{-(i/2)\int_{\Sigma}fg} e^{-(1/2)\int_{\Sigma}g\hat{m}g} \\
 &\times e^{-(1/4)\int_{\Sigma}(f-i\hat{m}g)B(f-i\hat{m}g)}.
 \end{aligned} \tag{3.24}$$

That is,

$$\begin{aligned}
 e^{-(1/4)\int_{\Sigma}(fBf-gDg+2fAg)} &= e^{-(i/2)\int_{\Sigma}fg} e^{-(1/2)\int_{\Sigma}g\hat{m}g} e^{-(1/4)\int_{\Sigma}fBf} \\
 &\times e^{(1/4)\int_{\Sigma}(\hat{m}g)(B\hat{m}g)} e^{(i/2)\int_{\Sigma}(\hat{m}g)(Bf)},
 \end{aligned} \tag{3.25}$$

where we have used the first relation in Eq. (2.10) to obtain the last term. Since Eq. (3.25) has to be valid for all g and f in K , then we have that

$$-\int_{\Sigma} fAg = i \int_{\Sigma} (\hat{m}g)(Bf) - i \int_{\Sigma} fg \tag{3.26}$$

and

$$\int_{\Sigma} gDg = \int_{\Sigma} (\hat{m}g)(B\hat{m}g) - 2 \int_{\Sigma} g\hat{m}g. \tag{3.27}$$

Using the first relation in Eq. (2.10), Eq. (3.26) can be rewritten as

$$\int_{\Sigma} f(A + iB\hat{m} - i\mathbf{1})g = 0. \tag{3.28}$$

In order to find \hat{m} , we will assume that $iB\hat{m} - i\mathbf{1}$ is a linear operator. Given that A is linear, then $L := A + iB\hat{m} - i\mathbf{1}$ is also linear. Equation (3.28) should be valid for all f and g in K , then $Lg = 0$ for all g in K (i.e., the kernel of the operator L is all of K), therefore $L = 0$ and

$$\hat{m} = B^{-1} + iB^{-1}A. \tag{3.29}$$

Note that \hat{m} is (i) a linear operator from K to $K \oplus iK$ and (ii) symmetric with respect to the inner product on K , $(f, g) = \int_{\Sigma} fg$, in the sense that $(g, B^{-1}g') = (B^{-1}g, g')$ and $(g, B^{-1}Ag') = (B^{-1}Ag, g')$ for all g and g' in K .

Equation (3.27) is simply a compatibility equation. If we substitute Eq. (3.29) on the RHS of Eq. (3.27), we get (using the fact that \hat{m} is symmetric)

$$\begin{aligned}
 &\int_{\Sigma} g(B^{-1} + iB^{-1}A)(\mathbf{1} + iA)g - 2 \int_{\Sigma} g(B^{-1} + iB^{-1}A)g \\
 &= - \int_{\Sigma} g(B^{-1} + B^{-1}A^2)g = \int_{\Sigma} gDg,
 \end{aligned} \tag{3.30}$$

where the last equation follows from the first relation in Eq. (2.8), which implies that $D + B^{-1}A^2 = -B^{-1}$ and therefore $B^{-1} + B^{-1}A^2 = -D$.

Substituting Eq. (3.29) in Eq. (3.20), we get \hat{M} . Thus, the representation of the operator $\hat{\pi}[g]$, for the general case of arbitrary complex structure (2.7), is given by

$$\hat{\pi}[g] \cdot \Psi[\varphi] = -i \int_{\Sigma} \left(g \frac{\delta}{\delta\varphi} - \varphi(B^{-1} + iB^{-1}A)g \right) \Psi[\varphi], \tag{3.31}$$

which can be rewritten in terms of the operator C , because from the third relation in Eq. (2.8) it follows that $B^{-1}A = -CB^{-1}$ and consequently

$$\hat{\pi}[g] \cdot \Psi[\varphi] = -i \int_{\Sigma} \left(g \frac{\delta}{\delta\varphi} - \varphi(B^{-1} - iCB^{-1})g \right) \Psi[\varphi]. \tag{3.32}$$

To summarize, we have used the vacuum expectation value condition (3.9) 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 Σ into 4M . 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 led to the ‘‘one-particle Hilbert space’’ had to be encoded in both of them. We have shown that the most natural way to use this information as conditions on the Schrödinger representation was through the condition (3.9) on the vacuum expectation values of the basic operators. This is the nontrivial input in the construction.

Before ending this section, several remarks are in order.

(i) Quantum configuration space. In the introduction of Sec. III we made the distinction between the classical configuration space \mathcal{C} of initial configurations $\varphi(x)$ of compact support and the quantum configuration space $\bar{\mathcal{C}}$. So far we have not specified $\bar{\mathcal{C}}$. In the case of Minkowski spacetime and flat embeddings, where Σ is a Euclidean space, the quantum configuration space is the space \mathcal{J}^* of tempered distributions on Σ . However, in order to define this space one uses the linear and Euclidean structure of Σ and it is not trivial to generalize it to general curved manifolds. These subtleties are outside the scope of this paper.

(ii) Gaussian nature of the measure. Note that the form of the measure given by Eq. (3.13) is always Gaussian. This is guaranteed by the fact that the operator B is positive definite in the ordinary L^2 norm on Σ , whose proof is given in [15].

However, the particular realization of the operator B will be different for different embeddings T_i of Σ [cf. Eq. (2.11)]. Thus, for a given J , the explicit form of the Schrödinger representation depends, of course, on the choice of embedding.

(iii) Hermiticity. In order to have a consistent quantization, one has to ensure that the operators associated to the basic (real) observables satisfy the “reality conditions,” which in this case means that they should be represented by Hermitian operators. It is straightforward to show that the operator given by Eq. (3.32) is indeed Hermitian.

(iv) Flat embedding in Minkowski spacetime. Let us now consider the most common and simple case, where the complex structure is chosen to yield the standard positive-negative frequency decomposition. This choice is associated to a constant vector field t^a . Furthermore, Σ is chosen to be the (unique) normal to t^a , namely the inertial frame in which the vector field t^a is “at rest.” Thus, the complex structure J is given by $J(\varphi, \pi) = (-(-\Delta + m^2)^{-1/2}\pi, (-\Delta + m^2)^{1/2}\varphi)$, which means that $A = C = 0$, $B = (-\Delta + m^2)^{-1/2}$, and $D = -(-\Delta + m^2)^{1/2}$. The quantum measure is then $d\mu = e^{-\int \varphi (-\Delta + m^2)^{1/2} \varphi} \mathcal{D}\varphi$. Thus, we recover immediately the Gaussian measure, existing in the literature [11,12], that corresponds to the usual Fock representation. As should be clear, this represents a very particular case (Minkowski spacetime and flat embeddings) of the general formulas presented in this section (valid for each globally hyperbolic spacetime and arbitrary embeddings).

It is illuminating to further compare the resulting Schrödinger representation with its Fock counterpart. This is done in [18].

IV. DISCUSSION

In this paper, we have constructed the Schrödinger representation for a scalar field on an arbitrary, globally hyperbolic spacetime. We have particularly emphasized the classical objects that need to be specified in order to have these representations. It is known that in the case of the Fock representation, formulated more naturally in a covariant setting, the only relevant construct is the complex structure J (or alternatively, as Wald chooses to emphasize, the metric μ); the infinite freedom in the choice of this object being precisely the ambiguity in the choice of quantum representation for the Fock Hilbert space. In the case of the functional representation, we have, in addition to J , a second classical construct, namely the choice of embedding of Σ . Even when one has a unique well-defined theory in the Fock language, the induced descriptions on two different embeddings T_1 and T_2 of Σ might not be (unitarily) equivalent. This second ambi-

guity was recently noted in [19]. This means that there might not be a unitary operator (that is, the evolution operator if one Σ_2 is to the future of the other surface Σ_1) that relates both Schrödinger descriptions. This apparently general feature of QFT on curved spacetimes has been recently confirmed in the quantum evolution of Gowdy T^3 cosmological models where the quantum description is reduced to a scalar field on a fixed expanding background [7,20].

We have used the algebraic formulation of quantum field theory to make precise the sense in which the Schrödinger representation can be unambiguously defined. In particular, the way in which the Fock representation is “Gaussian” in the functional language has been discussed in detail. We have noted that without some external input in the construction, such as the choice of a complex structure on the space of initial conditions, there is no *a priori* canonical way of finding a representation of the CCR; the reality-Hermiticity conditions are not enough to select the relevant representation and inner product. The exact implications of this result for full canonical quantum gravity are, in our opinion, still open. There are at least two aspects to this question. The first one has to do with the choice of the “physically relevant” inner product in full quantum gravity, namely when the theory does not reduce to a model field theory. The second aspect has to do with unitary evolution in general. In particular, it is not clear whether a lack of unitary evolution and the existence of the Schrödinger representation is a serious enough obstacle to render the theory useless. This possibility has been analyzed previously by several authors [21,7,20].

We hope that the material presented here will be of some help in setting the language for the task of understanding the fine issues of finding the “right” representation for, say, mid-superspace models in quantum gravity [5–7], and quantum gravity at large. In particular, these issues on nonunitarily related measures have emerged in the low-energy limit of semiclassical loop quantum gravity and its relation to Fock structures [22]. It is important to understand these results from the broader perspective of curved spacetime [23].

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