Dirac quantization of parametrized field theory

Madhavan Varadarajan[*]

Raman Research Institute, Bangalore 560 080, India
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Parametrized field theory (PFT) is free field theory on flat spacetime in a diffeomorphism invariant disguise. It describes field evolution on *arbitrary* (and in general, curved) foliations of the flat spacetime instead of only the usual flat foliations, by treating the "embedding variables" which describe the foliation as dynamical variables to be varied in the action in addition to the scalar field. A formal Dirac quantization turns the constraints of PFT into functional Schrödinger equations which describe evolution of quantum states from an arbitrary Cauchy slice to an infinitesimally nearby one. This formal Schrödinger picture-based quantization is unitarily equivalent to the standard Heisenberg picture-based Fock quantization of the free scalar field if scalar field evolution along arbitrary foliations is unitarily implemented on the Fock space. Torre and Varadarajan (TV) showed that for generic foliations emanating from a flat initial slice in spacetimes of dimension greater than 2, evolution is not unitarily implemented, thus implying an obstruction to Dirac quantization. We construct a Dirac quantization of PFT, unitarily equivalent to the standard Fock quantization, using techniques from loop quantum gravity (LQG) which are powerful enough to supercede the no-go implications of the TV results. The key features of our quantization include an LQG type representation for the embedding variables, embedding-dependent Fock spaces for the scalar field, an anomaly free representation of (a generalization of) the finite transformations generated by the constraints, and group averaging techniques. The difference between the 1 + 1-dimensional case and the case of higher spacetime dimensions is that for the latter, only finite gauge transformations are defined in quantum theory, not the infinitesimal ones.

I. INTRODUCTION

The usual description of quantum field theory on flat spacetime employs inertial coordinates. Such a description leads, naturally, to a study of quantum dynamics from one instant of inertial time to another. Each such instant corresponds to a flat spacelike Cauchy slice of the spacetime and the quantum dynamics evolves quantum fields between two such inertial slices. In contrast, in this work, we study aspects of quantum evolution of a free scalar field between two *arbitrary* (and in general, curved) Cauchy slices of the flat spacetime.

An elegant way to describe classical evolution of a free scalar field along arbitrary foliations of flat spacetime is through a formulation known as parametrized field theory (PFT). PFT is a free field theory on flat spacetime in a diffeomorphism invariant disguise [1]. Because of its general covariance and solvability, Kuchař pioneered the use of PFT as a toy model to study various issues which arise in canonical quantum gravity (see [1–3] and references therein). Our interest in PFT is, likewise, in its use as a toy model for quantum gravity.

PFT describes field evolution along arbitrary foliations of the flat spacetime by treating the "embedding variables" which describe the foliation as dynamical variables to be varied in the action in addition to the scalar field. Let $X^A := (T, X^1, \ldots, X^n)$ denote inertial coordinates on an $n + 1$-dimensional flat spacetime. In PFT, X^A are parame-

trized by a new set of arbitrary coordinates $x^\alpha = (t, x^1, \ldots, x^n)$ such that for fixed t, the embedding variables $X^A(t, x^1, \ldots, x^n)$ define a spacelike Cauchy slice of the flat spacetime. General covariance of PFT ensues from the arbitrary choice of x^α and implies that in its canonical description, evolution from one slice of an arbitrary foliation to another is generated by constraints.

The constraints of PFT in its Hamiltonian formulation take the form

$$C_A(x) := P_A(x) + h_A[\phi, \pi, X^B](x) = 0, \qquad (1.1)$$

where P_A and π are the momenta conjugate to X^A and ϕ, and h_A is related to the stress-energy of the scalar field. If we formally define $\hat{X}^A$ to act by multiplication and $\hat{P}_A$ by functional differentiation, we may attempt to construct a Dirac quantization in which the formal operator version of C_A acting on a physical state $|\Psi\rangle$ of the theory is given by

$$\left(\frac{1}{i} \frac{\delta}{\delta X^A} + \hat{h}_A\right)|\Psi\rangle = 0. \qquad (1.2)$$

Equation (1.2) takes the form of a functional Schrödinger equation which represents infinitesimal evolution of the quantum state $|\Psi\rangle$ from one Cauchy slice to another. The question of interest in this paper is whether a Dirac quantization of PFT yields a theory which is unitarily equivalent to the standard Fock quantization of the free scalar field on flat spacetime.

Note that the standard Fock representation is in the Heisenberg picture because the field operators are time dependent and the states are time independent. In contrast,

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*Electronic address: madhavan@rri.res.in

the representation used in (1.2) is one in which the operators $\hat{\phi}$, $\hat{\pi}$ commute with $\hat{X}^A$, $\hat{P}_A$ (in accordance with their classical Poisson brackets) and hence are embedding independent, whereas the states are embedding dependent. Thus, Dirac quantization leads to a Schrödinger picture-based representation. The Schrödinger and Heisenberg pictures are unitarily related if the evolution of the scalar field operators from some fixed initial Cauchy slice (this slice being the analog of the initial instant of time used to define the Schrödinger picture in quantum mechanics), to an arbitrary final Cauchy slice is unitarily implemented in the Heisenberg picture. If such an evolution is unitary, the Schrödinger picture can be defined as the "back-evolved" image of the Heisenberg picture.

Torre and Varadarajan (TV) [4] showed that in $1 + 1$ dimensions operator evolution is unitary, the functional Schrödinger picture exists as the unitary image of the standard Heisenberg picture-based Fock quantization, and the functional Schrödinger equation (1.2) is rigorously defined. However, for spacetimes of dimension greater than 2 and for generic choices of the final Cauchy slice, TV found that operator evolution from a flat initial slice is not unitarily implementable [5].[1] Thus the TV results seem to indicate an obstruction to a physically correct dirac quantization of higher dimensional PFT. If a Dirac quantization is not viable even in this simplest of models, it is a matter of concern for any Dirac quantization based approach to quantum gravity.

Recent results of Cho and Varadarajan [6] reinforce these apprehensions. They analyze the case of an axisymmetric scalar field evolving along arbitrary axisymmetric foliations of a flat $2 + 1$-dimensional spacetime. This system is equivalent, via Kuchař's canonical transformation [7], to the midisuperspace of cylindrically symmetric (1 polarization) gravitational fields. Reference [6] obtains a nonunitary result for generic axisymmetric scalar field evolution by showing that the action of generic radial diffeomorphisms on the scalar field operators is not unitarily implementable (see [6] for details).

One of the most active approaches to a Dirac quantization of gravity is loop quantum gravity (LQG). We are particularly interested in the implication of the results of [5,6] for LQG. Indeed, since a unitary representation of spatial diffeomorphisms lies at the heart of LQG, the results of [6] seem to be of significant concern. In this work, we show that these apprehensions are unjustified by constructing a Dirac quantization of PFT (in any spacetime dimension) which is unitarily equivalent to the standard Fock quantization. Our construction makes vital use of techniques developed in LQG (see [8] and references therein). Indeed, in the absence of these techniques, this work would not have been possible.

How do we avoid the negative implications of Refs. [5,6]? The key point is that LQG methods demand a Hilbert space representation for *all* the phase space variables, i.e. both the scalar field and the embedding variables. The arguments leading to Eq. (1.2) were based on a heuristic treatment of the embedding variables; $\hat{X}^A$, $\hat{P}_A$ were not defined as operators on a *Hilbert* space. As we shall see, once the correct Hilbert space representation is defined for the embedding variables, it is possible to construct a viable Dirac quantization. Specifically, we define an LQG type of representation on a nonseparable Hilbert space for the embedding sector. This enables us to specify embedding-dependent Fock space representations for the matter sector. The resultant nonseparable Hilbert space for the embedding and the matter field operators is called the kinematic Hilbert space in LQG terminology. It provides an anomaly free, unitary representation for a certain generalization of the *finite* (as opposed to infinitesimal) transformations generated by the constraints. Using group averaging techniques from LQG [8,9] one can construct physical states from kinematic ones. The physical Hilbert space, $\mathcal{H}_{\text{phys}}$, contains those states which are invariant under the unitary action of the "exponentiated" constraints and comes with a natural inner product as a result of group averaging. It can then easily be seen that the resulting representation of Dirac observables is such that the theory is unitarily equivalent to the standard Fock quantization.

Although the construction is valid for any dimension, it turns out that in higher dimensions only the finite transformations generated by the constraints (more precisely, their generalization, referred to above) can be defined in the quantum theory. This is in contrast to the $1 + 1$ case where, in a precise sense, infinitesimal transformations can also be defined. The nonexistence of these infinitesimal transformations in higher dimensions is the key feature of our quantization which allows us to avoid the (potential) obstructions to Dirac quantization indicated by the TV results. Since these infinitesimal transformations are ill defined, Eq. (1.2) is ill defined, and the subsequent arguments based on it are inapplicable.

We emphasize that (for higher dimensions), we do *not* provide a representation for the matter variables in which *evolution* from one arbitrary Cauchy slice to another is a unitary transformation. Instead, we construct a representa-

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[1]We refer the reader to [5] for a detailed proof of the TV result. Here we only mention that the choice of the final slice is by no means pathological. Indeed our view of this unexpected result is that it is unexpected purely on the basis of a faulty intuition which presupposes the triviality of all issues in free quantum field theory on flat spacetime. In contrast, intuition developed from the representation theory of infinite dimensional *field* theoretic systems, immediately points to the ubiquity of inequivalent representations. Indeed the TV results can also be viewed as asserting the existence of inequivalent Heisenberg picture-based quantizations of flat spacetime free quantum field theory. From this perspective, the standard "flat slice" based quantization is physically preferred because its choice of underlying complex structure (i.e. positive-negative frequency decomposition) is Poincaré *invariant*.

tion on which (a suitable generalization of) the finite transformations generated by the constraints act unitarily. Although related, the two sets of transformations, namely, those generated by the *constraints* on the phase space of PFT and those corresponding to *evolution* of the scalar field from one fixed slice to another, are distinct from each other. While the former act not only on the scalar field variables but also on the embedding variables, X^A, P^A, in the latter, the initial and final embeddings are fixed and the embedding momenta P^A do not even enter the description. In other words, the first set of transformations are pertinent to the description provided by PFT wherein the embeddings are also dynamical variables whereas the second refer to free scalar field evolution between two fixed, externally prescribed (though arbitrary) embeddings. Consequently the Hilbert spaces underlying the two quantum descriptions[2] are also distinct in that the one for PFT also provides a representation of the embedding variables whereas the standard Fock representation only attempts at providing a representation of the scalar field variables, with the embeddings playing the role of *c*-numbers. Hence a unitary representation of the finite transformations generated by the constraints on the former can, in principle, coexist with the lack of a unitary representation of free scalar field evolution on the latter. This (modulo the generalization of the finite transformations generated by the constraints alluded to above) is precisely what happens in our work.

As a consequence of this coexistence in the context of our quantization, Eq. (1.2) cannot be interpreted as an equation defining functional evolution of quantum states in a functional Schrödinger picture; indeed (1.2) is not even well defined (if, in the context of our specific quantization of PFT, (1.2) were to be well defined in such a way as to permit its interpretation as a functional Schrödinger equation encoding infinitesimal unitary evolution, the arguments subsequent to (1.2) would imply a contradiction with the TV results).

We proceed as follows. In Sec. II we provide a brief review of PFT. In Sec. III, we specify the representation for the embedding variables. In Sec. IV, we define the representation for the matter variables. This completes the specification of the kinematic Hilbert space. In Sec. V we show that there is a problem with our choice of operators depending on the embedding momenta[3] and arrive at an improved choice of operators. These operators are the quantum correspondents of the finite canonical transfor-

mations generated by the constraints. We show that these operators have a unitary action on the kinematic Hilbert space. Next, in Sec. VI, we complete the Dirac quantization by constructing the physical Hilbert space through group averaging. We display the action of Dirac observables on $\mathcal{H}_{phys}$ and demonstrate unitary equivalence with the standard Fock representation. We also show how to obtain the functional Schrödinger equation in $1 + 1$ dimensions where a suitable infinitesimal version of the unitary action of Sec. V can be defined. Section VII is devoted to a discussion of our results. In particular we discuss the existence of inequivalent (Dirac) quantizations in higher dimensions (this is the true implication of the TV results) and the presence of the Virasoro anomaly in $1 + 1$ dimensions even though the algebra of the unitary transformations of Sec. V is anomaly free (this discussion is essentially a reminder of the comments of Kuchař in [3] and of Kuchař and Torre in [11]).

In what follows, we use units in which $\hbar = c = 1$.

II. REVIEW OF PARAMETRIZED FIELD THEORY

In this section we provide a brief review of PFT. The reader may consult [1] for details.

A. The action for PFT

PFT is free scalar field theory on a fixed $n + 1$-dimensional flat spacetime written in a diffeomorphism invariant manner as follows. The action for a free scalar field ϕ on a fixed flat spacetime in terms of global inertial coordinates X^A, $A = 0, \ldots, n$ is

$$S_0[\phi] = -\frac{1}{2} \int d^{n+1}X \eta^{AB} \partial_A \phi \partial_B \phi, \qquad (2.1)$$

where the Minkowski metric in inertial coordinates, η^{AB}, is diagonal with entries $(-1, 1, 1 \ldots 1)$. If instead, we use coordinates x^α, $\alpha = 0, \ldots, n$ (so that X^A are "parametrized" by x^α, $X^A = X^A(x)$), we have

$$S_0[\phi] = -\frac{1}{2} \int d^{n+1}x \sqrt{\eta} \eta^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi, \qquad (2.2)$$

where $\eta_{\alpha\beta} = \eta_{AB} \partial_\alpha X^A \partial_\beta X^B$ and η denotes the determinant of $\eta_{\alpha\beta}$. The action for PFT is obtained by considering the right-hand side of (2.2) as a functional, not only of ϕ, but also of $X^A(x)$, i.e. $X^A(x)$ are considered as $n + 1$ new scalar fields to be varied in the action ($\eta_{\alpha\beta}$ is a function of $X^A(x)$). Thus

$$S_{PFT}[\phi, X^A] = -\frac{1}{2} \int d^{n+1}x \sqrt{\eta(X)} \eta^{\alpha\beta}(X) \partial_\alpha \phi \partial_\beta \phi.$$
$$(2.3)$$

Note that S_{PFT} is a diffeomorphism invariant functional of the scalar fields $\phi(x)$, $X^A(x)$. A variation of ϕ yields the equation of motion $\partial_\alpha(\sqrt{\eta} \eta^{\alpha\beta} \partial_\beta \phi) = 0$, which is just the flat spacetime equation $\eta^{AB} \partial_A \partial_B \phi = 0$ written in the co-

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[2]By this we mean the *kinematic* Hilbert space for PFT and the standard Fock space for the free scalar field. The *physical* Hilbert space in our Dirac quantization of PFT will be shown to be equivalent to the standard Fock space for the free scalar field.

[3]This problem can be traced to the fact that the requirement that each embedding must define a spacelike slice is in contradiction with a vector space structure on the space of embeddings. It is the analog of the problem of preserving the nondegeneracy of the spatial metric in quantum geometrodynamics [10].

ordinates x^α. On varying X^A, one obtains equations which are satisfied if $\eta^{AB}\partial_A\partial_B\phi = 0$. This implies that $X^A(x)$ are $n+1$ undetermined functions (subject to the condition that the determinant of $\partial_\alpha X^A$ is nonvanishing). This $n+1$-function worth of gauge is a reflection of the $n+1$-dimensional diffeomorphism invariance of S_{PFT}. Clearly the dynamical content of S_{PFT} is the same as that of S_0; it is only that the diffeomorphism invariance of S_{PFT} naturally allows a description of the standard free field dynamics dictated by S_0 on *arbitrary* foliations of the fixed flat spacetime.

B. Hamiltonian formulation of PFT

In the previous subsection, $X^A(x)$ had a dual interpretation—one as dynamical variables to be varied in the action, and the other as inertial coordinates on a flat spacetime. In what follows we shall freely go between these two interpretations.

We set $x^0 = t$ and $\{x^\alpha\} = \{t, x^a, a = 1, \ldots, n\}$. We restrict attention to $X^A(x)$ such that for any fixed t, $X^A(t, x^a)$ describe an embedded spacelike hypersurface in the $n+1$-dimensional flat spacetime (it is for this reason that $X^A(x)$ are called embedding variables in the literature). This means that, for fixed t, the functions $X^A(x)$ must be such that the symmmetric form q_{ab} defined by

$$q_{ab}(x) := \eta_{AB}\frac{\partial X^A(x)}{\partial x^a}\frac{\partial X^B(x)}{\partial x^b} \qquad (2.4)$$

is an n-dimensional Riemannian metric. This follows from the fact that $q_{ab}(x)$ is the induced metric on the hypersurface in the flat spacetime defined by $X^A(x)$ at fixed t.

An $n+1$ decomposition of S_{PFT} with respect to the time "t," leads to its Hamiltonian form:

$$S_{PFT}[\phi, X^A; \pi, P_A; N^A] = \int dt \int d^n x (P_A \dot{X}^A + \pi\dot\phi \\ - N^A C_A). \qquad (2.5)$$

Here π is the momentum conjugate to the scalar field ϕ, P_A are the momenta conjugate to the embedding variables X^A, and N^A are Lagrange multipliers for the first class constraints C_A, with $\{C_A, C_B\} = 0$. The constraints are functions on phase space which are linear in the embedding momenta, $C_A := P_A - h_A(X, \phi, \pi)$, where h_A are related to certain components of the stress-energy tensor of the scalar field on the $t = $ constant spatial hypersurface $X^A(t, x^a)$. It turns out that the motions on phase space generated by the "smeared" constraints, $\int d^n x (N^A C_A)$ correspond to scalar field evolution along arbitrary foliations of the flat spacetime, each choice of foliation being in correspondence with a choice of multipliers N^A. Since the constraints are first class they also generate gauge transformations, and as in general relativity, the notions of gauge and evolution are intertwined.

For future reference, we note that if we choose to smear the constraints with functions of the embedding variables,

the Poisson bracket algebra of the smeared constraints is isomorphic to the Lie algebra of diffeomorphisms on the spacetime manifold. We denote the spacetime manifold by M. Unless otherwise specified, we shall assume that M is diffeomorphic to R^{n+1}. Consequently, we shall also assume, unless otherwise specified, that the Cauchy slices are diffeomorphic to R^n so that x^a are global coordinates on R^n. We refrain from specifying boundary conditions/asymptotic conditions of various phase space variables and smearing functions; we anticipate that this can easily be done and will not alter any of our results.

Let ξ_1^A, ξ_2^A be two vector fields on M. We denote their dependence on the inertial coordinates X^A by $\xi_I^A = \xi_I^A(X) I = 1, 2$. These vector fields define the two sets of functions of the embedding variables, $\xi_I^A(X(x))$, $I = 1, 2$, in an obvious manner. We smear the constraints with these functions to get $C(\xi_I) = \int d^n x(\xi_I^A C_A)$, $I = 1, 2$. The smeared constraints have the algebra

$$\{C(\xi_1), C(\xi_2)\} = C(\mathcal{L}_{\xi_2}\xi_1), \qquad (2.6)$$

where $\mathcal{L}_{\xi_2}\xi_1^A = \xi_2^B\frac{\partial\xi_1^A}{\partial X^B} - \xi_1^B\frac{\partial\xi_2^A}{\partial X^B}$. Clearly, Eq. (2.6) displays an isomorphism with the Lie bracket between vector fields on M. The latter define the Lie algebra of diffeomorphisms on M by virtue of the fact that the diffeomorphisms (connected to identity) on M are generated by vector fields on M.

Given a vector field ξ^A, we define, as before, the smeared constraint $C(\xi)$ by

$$C(\xi) := \int d^n x \xi^B(X(x)) C_B(x). \qquad (2.7)$$

Then it is easy to see that

$$\{X^A(x), C(\xi)\} = \xi^A(X(x)) = \xi^B\frac{\partial X^A}{\partial X^B} =: \mathcal{L}_\xi X^A. \qquad (2.8)$$

In terms of structures on M, the above equation has the following interpretation: ξ. ξ generates a 1 parameter family of diffeomorphisms $d_\xi(t):M \to M$. Any diffeomorphism on M maps the hypersurface $X^A(x)$ to another hypersurface in M. The new embedding defined by the infinitesimal action of $d_\xi(t)$ on $X^A(x)$ corresponds to that defined by Eq. (2.8) above.

It is also easy to see that

$$\{\phi(x), C(\xi)\} = \left\{\phi(x), \int d^n x \xi^A(X(x)) h_A(x)\right\}, \qquad (2.9)$$

$$\{\pi(x), C(\xi)\} = \{\pi(x), \int d^n x \xi^A(X(x)) h_A(x)\}. \qquad (2.10)$$

It is straightforward to verify that the right-hand side of the above equations has the following interpretation in terms of free scalar field evolution on M. Let $(\phi(x), \pi(x))$ be initial data on the Cauchy slice defined by $X^A(x)$. Consider the evolution of this data, via the free scalar field equations on M, to the infinitesimally nearby slice defined by

Eq. (2.8). The evolved data correspond to that defined by the right-hand sides of (2.9) and (2.10) above.

C. The standard Fock representation via gauge fixing

A gauge fixing of the constraints which maps the classical theory directly onto the standard description of a free scalar field in inertial coordinates is, not surprisingly, $X^1 = x^1, \ldots, X^n = x^n, X^0 = t$.[4] It is straightforward to implement this gauge fixing, eliminate the embedding momenta, and obtain a reduced action identical to (the Hamiltonian form of) S_0 (2.1). As is well known, this form of the theory admits the standard Fock quantization wherein quantum states $|\Psi\rangle$ are time independent and the field operators $\hat{\phi}(x, t)$ are time dependent (note that, here, (x, t) are chosen to be inertial coordinates by virtue of the gauge fixing conditions).

It is also possible to obtain the standard Fock quantization by first subjecting the canonical coordinates X^A, P_A, ϕ, π to a Hamilton-Jacobi type of canonical transformation and then constructing a Dirac quantization [1,3]. In this work we are interested in a direct Dirac quantization of PFT without any canonical transformations to simplify the constraints. This is because we are interested in PFT as a toy model for gravity and no such simplifying canonical transformation is known for gravity.

III. THE REPRESENTATION OF THE EMBEDDING VARIABLES

We construct the representation for the embedding variables through the following steps. First we specify a complete set of functions on the embedding phase space which is closed under Poisson brackets and under complex conjugation. By complete, it is meant that any other function on this phase space can be written as the (limit) of sums and products of these functions.

Next, we define a representation of these functions as quantum operators so that the Poisson brackets go to quantum commutators. Finally, we specify an inner product on the representation space such that the relations implied by complex conjugation are enforced as adjointness relations on the operators.

As is conventional in Hamiltonian theory, we shall drop the explicit dependence of various variables on the time coordinate t. Thus, the notation $f(x)$ signifies the functional dependence of the function f on the coordinates x^a.

A. The classical Poisson bracket algebra

Let $G^A(x)$, $A = 0, \ldots, N$ be smooth functions of x^a, $a = 1, \ldots, n$. We define the functional, H_G, of the embedding momenta as follows:

[4]Technically, this is not a gauge fixing but a 1 parameter family of gauge fixings (one for each value of t) known as "deparametrization."

$$H_G[P_A] = \exp i \int d^n x \, G^B P_B. \tag{3.1}$$

We shall choose our complete set of functions as $(X^A(x), H_G[P_A])$ of functions $(X^A(x), H_G[P_A])$. It is easy to check that the only nontrivial Poisson brackets are

$$\{X^A(x), H_G\} = iG^A(x)H_G. \tag{3.2}$$

The set of functions is also closed under complex conjugation since

$$(X^A(x))^* = X^A(x) \quad (H_G)^* = H_{-G}. \tag{3.3}$$

B. The representation

We specify the representation of our set of functions as quantum operators by defining their action on basis states of our representation. Each state in the basis is labeled by a set of smooth functions of x^a, $a = 1, \ldots, n$. Given the set of smooth functions, $F^A(x)$ $A = 0, \ldots, N$, we denote the corresponding basis state by $|F\rangle$. We define the action of $\hat{X}^A$, $\hat{H}_G$ through

$$\hat{X}^A(x)|F\rangle = F^A(x)|F\rangle, \tag{3.4}$$

$$\hat{H}_G|F\rangle = |F - G\rangle. \tag{3.5}$$

It is easy to verify that the above equations provide a representation of the classical Poisson bracket relations.

C. Inner product

Given the smooth functions $F_1^A(x)$, $F_2^A(x)$, we define the *Kronecker* delta function δ_{F_1, F_2} by

$$\delta_{F_1, F_2} = 0 \text{ if there exists } A, x^a \text{ such that } F_1^A(x) \neq F_2^A(x)$$
$$= 1 \text{ if } F_1^A(x) = F_2^A(x) \text{ for all } A, x^a. \tag{3.6}$$

Then the inner product between two states in our basis labeled by the smooth functions $F_1^A(x)$, $F_2^A(x)$ is defined to be

$$\langle F_1 | F_2 \rangle = \delta_{F_1, F_2}. \tag{3.7}$$

Note that this inner product implies that our basis states are orthonormal. Since the basis states are uncountable, we have a nonseparable representation space. Also note that, with this inner product, $\hat{H}_G$ does not have the appropriate continuity in $G^A(x)$ to define $\hat{P}_A(x)$; thus although $\hat{H}_G$ is a well-defined operator, this representation does not allow the existence of $\hat{P}_A(x)$.

It suffices to check the implementation of the "reality conditions" (3.3) in the context of pairs of basis states, i.e. it is straightforward to verify that

$$(\langle F_1 | \hat{X}^A(x) F_2 \rangle)^* = \langle F_2 | \hat{X}^A(x) F_1 \rangle, \tag{3.8}$$

$$(\langle F_1 | \hat{H}_G F_2 \rangle)^* = \langle F_2 | \hat{H}_{-G} F_1 \rangle. \tag{3.9}$$

For our purposes in subsequent sections we could stop here. However, for completeness, we specify the obvious steps for the construction of the Hilbert space and complete verification of the reality conditions thereon.

We define the set $\mathcal{D}_X$ to be the set of finite linear combinations of the basis states defined above. Thus $|\psi\rangle \in \mathcal{D}_X$ if

$$|\psi\rangle = \sum_{I=1}^{N} a_I |F_I\rangle, \qquad (3.10)$$

where $F_I^A(x)$, $I = 1, \ldots, N$ are smooth functions such that $F_I^A(x) = F_J^A(x)$ only when $I = J$, N is finite and a_I, $I = 1, \ldots, N$ are complex numbers. The inner product (3.7) can be extended to $\mathcal{D}_X$ by appropriate linearity. $\mathcal{D}_X$ serves as a dense set for the embedding sector Hilbert space $\mathcal{H}_X$, i.e. the Cauchy completion of $\mathcal{D}_X$ in the inner product (3.7) yields $\mathcal{H}_X$. Thus $|\psi\rangle \in \mathcal{H}_X$ if

$$|\psi\rangle = \sum_{I=1}^{\infty} a_I |F_I\rangle, \qquad (3.11)$$

where $F_I^A(x)$ are smooth functions such that $F_I^A(x) = F_J^A(x)$ only when $I = J$ and $\sum_{I=1}^{\infty} |a_I|^2 < \infty$. Note that $\mathcal{D}_X$ serves as a dense domain for the unbounded operator $\hat{X}^A(x)$.

IV. THE REPRESENTATION FOR THE SCALAR FIELD VARIABLES

A. Preliminary remarks

The only nontrivial Poisson bracket involving $\phi(x)$ and/or $\pi(x)$ is $\{\phi(x), \pi(y)\} = \delta(x, y)$. In particular we have the trivial Poisson brackets $\{\phi(x), P_A(y)\} = 0$ and $\{\pi(x), P_A(y)\} = 0$ which are equivalent to the equations $\frac{\delta\phi(x)}{\delta X^A(y)} = 0$ and $\frac{\delta\pi(x)}{\delta X^A(y)} = 0$. As a result of the latter equations, we seek, in quantum theory, a representation of $\hat{\phi}(x)$, $\hat{\pi}(x)$ which is independent of the embeddings. This is like the Schrödinger picture in standard quantum mechanics, with (the eigenvalues of) $\hat{X}^A(x)$ playing the role of time. Bearing this analogy in mind, we shall pattern our constructions below on corresponding structures in standard quantum mechanics.

In usual particle quantum mechanics, the Schrödinger picture is constructed by evolving the Heisenberg picture operators at time t back to some fixed initial time t_0, usually chosen to be $t_0 = 0$. Here, in order to make contact with [4,5] we choose the analog of $t_0 = 0$ to be the initial flat embedding $F_0^A(x) = (0, x^1, \ldots, x^n)$. Thus, we want $\hat{\phi}(x)$, $\hat{\pi}(x)$ to act as if they were Heisenberg picture fields at the initial embedding $F_0^A(x)$. This prompts the definitions

$$\hat{\phi}(x) = \frac{1}{(2\pi)^{n/2}} \int \frac{d^n k}{\sqrt{2k}} (\hat{a}_S(k) e^{i\vec{k}\cdot\vec{x}} + \hat{a}_S^\dagger(k) e^{-i\vec{k}\cdot\vec{x}}), \quad (4.1)$$

$$\hat{\pi}(x) = \frac{1}{(2\pi)^{n/2}} \int \frac{d^n k \sqrt{k}}{\sqrt{2}} (-i\hat{a}_S(k) e^{i\vec{k}\cdot\vec{x}} + i\hat{a}_S^\dagger(k) e^{-i\vec{k}\cdot\vec{x}}), \qquad (4.2)$$

where we have denoted $(x^1, \ldots, x^n)$, $(k^1, \ldots, k^n)$ by $\vec{x}$, $\vec{k}$ and where $k := \sqrt{\vec{k} \cdot \vec{k}}$. If evolution is unitary, the Schrödinger and Heisenberg picture representations exist on the same Hilbert space. If this were the case, we could define $\hat{a}_S(k)$, $\hat{a}_S^\dagger(k)$ in the usual way as annihilation and creation operators. We could then generate the Fock space by the action of the creation operators on the standard Fock vacuum. Since for spacetime dimensions greater than 2 (i.e. for $n > 1$) generic evolution is not unitary [5], this is *not* the case and, instead, we define the action of $\hat{a}_S(k)$, $\hat{a}_S^\dagger(k)$ in analogy with the following structure in usual quantum mechanics.

B. The Heisenberg and Schrödinger pictures in standard quantum mechanics

Consider a system with phase space coordinatized by (complex) canonical coordinates (a, a^*) so that $\{a, a^*\} = -i$. Let its dynamics be described by some time dependent quadratic Hamiltonian. Consequently, classical evolution is a linear canonical transformation so that

$$a(t_2) = \alpha(t_2, t_1) a(t_1) + \beta(t_2, t_1) a^*(t_1), \qquad (4.3)$$

where α, β are complex functions (of the initial and final times t_1 and t_2) which are determined by the Hamiltonian of the system. Denoting the pair a, a^* by $\vec{a}$ and defining the matrix $C(t_2, t_1)$ by

$$C(t_2, t_1) = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}, \qquad (4.4)$$

we can write Eq. (4.3) as

$$\vec{a}(t_2) = C(t_2, t_1)\vec{a}(t_1). \qquad (4.5)$$

For future purposes we note that Eq. (4.5) implies the identities:

$$C(t_3, t_1) = C(t_3, t_2) C(t_2, t_1), \qquad C(t, t) = \mathbf{1}, \qquad (4.6)$$

where $\mathbf{1}$ denotes the identity operator. In the Heisenberg picture, $a(t)$, $a^*(t)$ are represented by the operators $\hat{a}_H(t)$, $\hat{a}_H^\dagger(t)$. The time independent state space is generated by the action of the creation operator, $\hat{a}_H^\dagger(0)$, on the vacuum $|0\rangle$, the vacuum being defined by $\hat{a}_H(0)|0\rangle = 0$. Clearly, $\hat{a}_H(t)$, $\hat{a}_H^\dagger(t)$ are related to the $t = 0$ operators through the relation

$$\vec{\hat{a}}_H(t) = C(t, 0)\vec{\hat{a}}_H(0), \qquad (4.7)$$

where we have used the obvious notation that $\vec{\hat{a}}_H(t)$ denotes the pair $\hat{a}_H(t)$, $\hat{a}_H^\dagger(t)$.

Let the unitary transformation corresponding to evolution from t_1 to t_2 be denoted by $U(t_2, t_1)$. Then the Schrödinger picture representative of $\vec{a}(t)$ is given by

$$\vec{a}_S = U^\dagger(t,0)\vec{a}_H(t)U(t,0) = \vec{a}_H(0) \qquad (4.8)$$

and the Schrödinger picture "vacuum" is given by

$$|0,t\rangle_S = U^\dagger(t,0)|0\rangle. \qquad (4.9)$$

Clearly, the Schrödinger vacuum is annihilated by the operator

$$\hat{b}(t) = U^\dagger(t,0)\vec{a}_H(0)U(t,0) = U^\dagger(t,0)\vec{a}_S U(t,0) \quad (4.10)$$

and the Schrödinger picture image of the Heisenberg state $(\hat{a}_H^\dagger(0))^n|0\rangle$ is the state $(\hat{b}^\dagger(t))^n|0,t\rangle_S$. Note that the Schrödinger picture image of Eq. (4.7) is

$$\vec{a}_H(0) = \vec{a}_S = C(t,0)\vec{b}(t), \qquad (4.11)$$

which, in conjunction with Eq. (4.6), implies that

$$\hat{b}(t) = C(0,t)\vec{a}_S. \qquad (4.12)$$

Given the operator $\vec{a}_S$, the above equation can be defined even in the absence of the unitary transformation $U(t,0)$ and hence can be used to define the representation in the field theory case.

C. Some considerations in classical field theory

Before we define the representation for the matter sector of PFT, it is useful to review the classical (field theoretic) structures which are in correspondence with the ones in Sec. IV B.

Consider free scalar field evolution from the slice defined by the embedding $F_1^A(x)$ to the slice defined by the embedding $F_2^A(x)$. Let the scalar field data on $F_I^A(x)$, $I = 1$, 2 be denoted by $(\phi(x), \pi(x)) = (\phi_{F_I}(x), \pi_{F_I}(x))$. Instead of the scalar field data, it is more convenient to work with the modes $a(\vec{k})$, $a^*(\vec{k})$ where

$$a(\vec{k}) = \frac{1}{(2\pi)^{n/2}} \int d^n x \sqrt{\frac{k}{2}}\left(\phi(x) + i\frac{\pi(x)}{k}\right)e^{-i\vec{k}\cdot\vec{x}}. \quad (4.13)$$

Thus $a(\vec{k})$, $a^*(\vec{k})$ are the classical correspondents of $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ defined in Eqs. (4.1) and (4.2).

When the data for the scalar fields is $(\phi(x), \pi(x)) = (\phi_{F_I}(x), \pi_{F_I}(x))$, we denote the corresponding evaluation of the modes $a(\vec{k})$, $a^*(\vec{k})$ by $a_{F_I}(\vec{k})$, $a_{F_I}^*(\vec{k})$. Explicitly,

$$a_{F_I}(\vec{k}) = \frac{1}{(2\pi)^{n/2}} \int d^n x \sqrt{\frac{k}{2}}\left(\phi_{F_I}(x) + i\frac{\pi_{F_I}(x)}{k}\right)e^{-i\vec{k}\cdot\vec{x}}. \tag{4.14}$$

As in (4.3), classical evolution is a linear canonical transformation so that

$$a_{F_2}(\vec{k}) = \int d^n l\, \alpha_{F_2,F_1}(\vec{k},\vec{l})a_{F_1}(\vec{l})$$
$$+ \int d^n l\, \beta_{F_2,F_1}(\vec{k},\vec{l})a_{F_1}^*(\vec{l}). \qquad (4.15)$$

The coefficients α, β satisfy the Bogoliubov conditions [12] by virtue of the transformation being canonical. In analogy to Sec. IV B, we denote the pair of functions $a_{F_I}(\vec{k})$, $a_{F_I}^*(\vec{k})$ by $\vec{a}(F_I)$ and define $C(F_2, F_1)$ to be the infinite dimensional matrix

$$C(F_2, F_1) = \begin{pmatrix} \alpha_{F_2,F_1}(\vec{k},\vec{l}) & \beta_{F_2,F_1}(\vec{k},\vec{l}) \\ (\beta_{F_2,F_1}(\vec{k},\vec{l}))^* & (\alpha_{F_2,F_1}(\vec{k},\vec{l}))^* \end{pmatrix}. \quad (4.16)$$

Then Eq. (4.15) can be written as

$$\vec{a}(F_2) = C(F_2, F_1)\vec{a}(F_1) \qquad (4.17)$$

and it follows that

$$C(F_3, F_1) = C(F_3, F_2)C(F_2, F_1), \qquad C(F, F) = \mathbf{1},$$
$$(4.18)$$

where, as in (4.6), $\mathbf{1}$ denotes the identity operator.

We can now define the Schrödinger picture as follows.

D. The representation for $\hat{\phi}(x)$, $\hat{\pi}(x)$

We denote $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ by $\vec{a}_S$. Given the slice $F^A(x)$, we define the operators $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k}) =: \vec{b}(F)$ through $\vec{b}(F) = C(F_0, F)\vec{a}_S$ (this is the counterpart of (4.12)). Then we have, analogous to Eq. (4.11), that

$$\vec{a}_S = C(F, F_0)\vec{b}(F). \qquad (4.19)$$

We define the Fock space $\mathcal{H}_F$ as the one for which $(\hat{b}_F(\vec{k}), \hat{b}_F^\dagger(\vec{k}))$ are annihilation and creation operators. We denote states in $\mathcal{H}_F$ by $|\psi, F\rangle$ and the vacuum state by $|0, F\rangle$ so that $\hat{b}_F(\vec{k})|0, F\rangle = 0$ for every $\vec{k}$.

Consider the (nonseparable) kinematic Hilbert space $\mathcal{H}_{\text{kin}}$ defined as

$$\mathcal{H}_{\text{kin}} = \bigoplus_F |F\rangle \otimes \mathcal{H}_F, \qquad (4.20)$$

where $|F\rangle$ carries the representation of the embedding operators as discussed in Sec. III. The linear sum of vector spaces is over all spacelike embeddings $F^A(x)$.[5] The inner product on $\mathcal{H}_{\text{kin}}$ is defined in the obvious way from the inner products on the embedding sector and on $\mathcal{H}_F$. To this end consider the linear subspace of $\mathcal{H}_{\text{kin}}$ denoted by $\mathcal{D}$ and defined as

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[5]This is akin to the sum over the uncountable label set of graphs in LQG [8]. Just as the set of spin network states organize themselves into a separable set of states associated with each graph label, here we have a separable Fock space associated with each embedding label.

$$\mathcal{D} = \left\{ |\psi\rangle : |\psi\rangle = \sum_{I=1}^{N} a_I |F_I\rangle \otimes |\psi_I, F_I\rangle \right\}, \qquad (4.21)$$

for all finite N and all choices of complex coefficients a_I. The inner product between $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{D}$ with $|\psi_i\rangle = \sum_{I=1}^{N} a_{iI} |F_I\rangle \otimes |\psi_{iI}, F_I\rangle$, $i = 1, 2$ is

$$(|\psi_1\rangle, |\psi_2\rangle) = \sum_{I=1}^{N} a_{1I}^* a_{2I} \langle \psi_{1I} F_I | \psi_{2I} F_I \rangle. \qquad (4.22)$$

$\mathcal{D}$ is dense in $\mathcal{H}_{\text{kin}}$, so that the latter can be obtained by the completion of the former in the above inner product.

On any basis element of the form $|F\rangle \otimes |\psi, F\rangle$, the operators $\hat{X}^A(x)$, $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ are defined through

$$\hat{X}^A(x)|F\rangle \otimes |\psi, F\rangle = F^A(x)|F\rangle \otimes |\psi, F\rangle, \qquad (4.23)$$

$$\hat{b}_F(\vec{k})|F\rangle \otimes |\psi, F\rangle = |F\rangle \otimes \hat{b}_F(\vec{k})|\psi, F\rangle, \qquad (4.24)$$

$$\hat{b}_F^\dagger(\vec{k})|F\rangle \otimes |\psi, F\rangle = |F\rangle \otimes \hat{b}_F^\dagger(\vec{k})|\psi, F\rangle, \qquad (4.25)$$

with $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ defined in terms of $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k})$ through Eq. (4.19).[6]

It can easily be verified, with these definitions, that $\hat{X}^A(x)$ commutes with $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$, $\hat{X}^B(y)$ and that $(\hat{X}^A(x))^\dagger = \hat{X}^A(x)$.

Note that since $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k})$ are annihilation and creation operators on the Fock space $\mathcal{H}_F$, they are adjoint to each other and have canonical commutation relations on $\mathcal{H}_F$. Note also that $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ map states in the subspace $|F\rangle \otimes \mathcal{H}_F \subset \mathcal{H}_{\text{kin}}$ into states in the same subspace. These facts, in conjunction with Eq. (4.19), the definition of the embedding sector inner product (3.7), and the fact that $C(F, F_0)$ is a Bogoliubov transformation, imply that $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ are adjoint to each other on $\mathcal{H}_{\text{kin}}$ and have the right commutation relations with each other.

From Eq. (4.19), the operators $\vec{\hat{a}}_S$ and $\vec{\hat{b}}(F)$ are related by the Bogoliubov transformation $C(F, F_0)$. The TV results imply that this Bogoliubov transformation is not unitarily implementable on $\mathcal{H}_F$ for generic choices of $F^A(x)$. Because of this fact, we are unsure if $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ are well-defined operators (after appropriate smearing (see Footnote 6)) on (a dense set in) $\mathcal{H}_{\text{kin}}$. However, the formal "working" definition of $\vec{\hat{a}}_S$ adopted above through Eqs. (4.19), (4.24), and (4.25), and the consequent satisfaction, at a formal level, of the reality conditions and com-

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[6]Here $|\psi, F\rangle \in \mathcal{H}_F$. We have glossed over the fact that $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k})$ are operator valued distributions when the Cauchy slices are noncompact. We have also glossed over the fact that even when appropriately smeared, $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k})$ are not bounded operators and hence only densely defined. We expect that these technicalities can easily be taken care of; in the interests of pedagogy, we refrain from a careful treatment of these mathematical niceties.

mutation relations involving $\vec{\hat{a}}_S$, filters down to the rigorous definition of Dirac observables in Sec. VI C which satisfy the correct commutation and adjointness relations on (a dense set in) $\mathcal{H}_{\text{kin}}$.[7]

To summarize, the representation for $\hat{X}^A(x)$, $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ on $\mathcal{H}_{\text{kin}}$ is such that

$$[\hat{X}^A(x), \hat{X}^B(y)] = 0, \qquad [\hat{X}^A(x), \vec{\hat{a}}_S] = 0, \qquad (4.26)$$

$$[\hat{a}_S(\vec{k}), \hat{a}_S(\vec{l})] = 0, \qquad [\hat{a}_S(\vec{k}), \hat{a}_S^\dagger(\vec{l})] = \delta(\vec{k}, \vec{l}), \quad (4.27)$$

$$(\hat{X}^A(x))^\dagger = \hat{X}^A(x), \qquad (\hat{a}_S(\vec{k}))^\dagger = \hat{a}_S^\dagger(\vec{k}). \qquad (4.28)$$

We have deliberately refrained from defining $\hat{H}_G$ to act in the obvious manner because there are problems with such an action. We now turn to a discussion (and resolution) of these problems.

V. PROBLEMS WITH $\hat{H}_G$ AND THEIR RESOLUTION IN TERMS OF A TREATMENT OF THE QUANTUM CONSTRAINTS

A. Problems with $\hat{H}_G$

We would like to define $\hat{H}_G$ in the obvious manner by $\hat{H}_G|F\rangle \otimes |\psi, F\rangle = |F - G\rangle \otimes |\psi, F\rangle$, but this has two problems. First, assuming $F^A(x) - G^A(x)$ is an embedding, if the representation of the matter operators on $\mathcal{H}_F$ is not unitarily equivalent to that on $\mathcal{H}_{F-G}$, the above state does not lie in $\mathcal{H}_{\text{kin}}$. Second, if $F^A(x)$ is an embedding, $F^A(x) - G^A(x)$ need not be an embedding because embeddings need to satisfy a nondegeneracy condition (described in Sec. II B; see Eq. (2.4) and the subsequent discussion) which ensures that they define a spatial slice in the spacetime M.

The first problem can be fixed by enlarging the Hilbert space to $\mathcal{H}_X \otimes \oplus_F \mathcal{H}_F$ (recall that $\mathcal{H}_X$ is defined in Sec. III B as the Hilbert space of the embedding sector). However the second problem is more acute and is a reflection of a similar problem in the quantization of configuration spaces which are not vector spaces, an important example being that of the space of all Riemannian metrics [10].

We avoid these problems by considering an alternative set of functions which we will promote to quantum operators. Thus, instead of choosing our basic Poisson algebra to be generated by the $H_G, X^A(x), \pi(x), \phi(x)$, we consider the alternative set of functions $C_A(x), X^A(x), \pi(x), \phi(x)$, where $C_A(x)$ are the constraints of PFT given by Eq. (1.1). From our previous work [5], we anticipate (for $n > 1$) that there are obstacles to define $\hat{C}_A(x)$ as operators. Therefore, motivated by the treatment of the quantum (spatial diffeomorphism) constraints in LQG [8], we adopt the following

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[7]We thank Guillermo Mena for discussions on this point.

strategy which focuses on the finite canonical transformations generated by $C_A(x)$ rather than on $C_A(x)$ itself.

First we consider the smeared constraints $C(\xi)$ defined by Eq. (2.7). From the discussion in Sec. II B (see Eqs. (2.8), (2.9), and (2.10)), we expect that every *finite* canonical transformation generated by $C(\xi)$ can be labeled by a corresponding spacetime diffeomorphism $d:M \rightarrow M$ where d is generated by the vector field ξ^A. The expected correspondence is as follows. d maps the point p in M with inertial coordinates X^A to the point $d(p)$. We denote the inertial coordinates of $d(p)$ by X_d^A and denote the image of the spatial slice $X^A(x)$ by d as $X_d^A(x)$. Then the action of the canonical transformation labeled by d is to map the embedding variables $X^A(x)$ to $X_d^A(x)$ and evolve the scalar field data $(\phi(x), \pi(x))$ to the data $(\phi_d(x), \pi_d(x))$, where $(\phi_d(x), \pi_d(x))$ are obtained from $(\phi(x), \pi(x))$ as follows. Consider the slice $X^A(x)$ in M. Let initial data on this slice be $(\phi(x), \pi(x))$. Evolve this data from the slice $X^A(x)$ to the slice $X_d^A(x)$ via the free scalar field evolution equations on the flat spacetime M. This evolved data on the slice $X_d^A(x)$ is $(\phi_d(x), \pi_d(x))$.

Note that the data $(X_d^A(x), \phi_d(x), \pi_d(x))$ (partially) specify a point in phase space only if $X_d^A(x)$ is also a spacelike slice. Thus, in order to preserve the phase space, we would like to restrict attention to those vector fields $\xi^A(X)$ which generate diffeomorphisms which preserve the spacelike property of the embeddings $X^A(x)$. Let the set of spacelike embeddings be $\mathcal{E}$. We denote by $\mathcal{G}(\mathcal{E})$, the subspace of diffeomorphisms $d:M \rightarrow M$ such that $X_d^A(x) \in \mathcal{E} \ \forall \ X^A(x) \in \mathcal{E}$. It is not clear to us if there exist any elements of $\mathcal{G}(\mathcal{E})$ which are not conformal isometries of the spacetime (M, η_{AB}).[8] The discussion in [13] indicates that the issue is not trivial. We return to it at the end of this section. For the moment we make the following assumption: $\mathcal{G}(\mathcal{E})$ exists as an infinite dimensional subgroup[9] of the group of diffeomorphisms and every $d \in \mathcal{G}(\mathcal{E})$ is generated by some vector field $\xi^A(X)$.

Consider the canonical transformation on phase space labeled by the diffeomorphism $d \in \mathcal{G}(\mathcal{E})$. We denote the operator which implements this transformation in quantum theory by $\hat{U}_d$. Then, in addition to the canonical commutation relations between $\hat{\phi}(x)$, $\hat{\pi}(x)$, $\hat{X}^A(x)$, we also need to represent $\hat{U}_d$ such that

$$\hat{U}_{d_2}\hat{U}_{d_1} = \hat{U}_{d_1 \circ d_2}, \tag{5.1}$$

$$\hat{U}_{d^{-1}} = \hat{U}_d^\dagger, \tag{5.2}$$

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[8]We thank Charles Torre for discussions on this point.

[9]We expect that the vanishing of the constraints $C_A(x)$ is equivalent to the vanishing of the smeared constraints $C(\xi)$ provided that the latter holds for sufficiently many $\xi^A(X)$. Since "sufficiently many" evidently includes "infinitely many," a minimal requirement on $\mathcal{G}(\mathcal{E})$ is that it be infinite dimensional.

$$\hat{U}_d\hat{X}^A(x)\hat{U}_d^\dagger = \hat{X}_d^A(x), \tag{5.3}$$

$$\hat{U}_d\hat{\phi}(x)\hat{U}_d^\dagger = \hat{\phi}_d(x), \tag{5.4}$$

$$\hat{U}_d\hat{\pi}(x)\hat{U}_d^\dagger = \hat{\pi}_d(x). \tag{5.5}$$

Several comments are in order. The fact that Eq. (5.1) defines a representation of $\mathcal{G}(\mathcal{E})$ by right multiplication follows from Eq. (2.6). Equation (5.2) follows from the fact that the constraints are real. The right-hand side of Eq. (5.3) is to be understood as follows. The action of d on the embedding $X^A(x)$ yields the d-dependent functionals (one for every value of A), $f_d^A[X; x)$, of the embedding. Here, in a notation introduced by Kuchař (see, for example, [7]), the left square bracket denotes the fact that for each value of A, f^A is a functional of the embedding and the round bracket denotes the fact that f^A is a function of x. Using our notation in the discussion above, we have $X_d^A(x) = f_d^A[X; x)$. Then by $\hat{X}_d^A(x)$ we mean that the embedding should be replaced by its corresponding quantum operator in $f_d^A[X; x)$, i.e. $\hat{X}_d^A(x) := f_d^A[\hat{X}; x)$. Finally, the right-hand sides of Eqs. (5.4) and (5.5) are to be understood in a similar manner. The classical fields $(\phi_d(x), \pi_d(x))$ are d-dependent functionals of the embeddings and the fields $(\phi(x), \pi(x))$. Since the underlying dynamics is that of a free field, it follows that the dependence on $(\phi(x), \pi(x))$ is linear. The right-hand sides of Eqs. (5.4) and (5.5) are obtained by substituting the embeddings and the matter fields by the corresponding quantum operators. Since the right-hand sides of (5.3), (5.4), and (5.5) are either independent of or linear in the matter fields, and independent of the embedding momenta operators, there are no operator ordering ambiguities in their definition.

Let d be generated by the vector field $\xi^A(X)$. Suppose that $\hat{U}_d$ has the appropriate continuity in d so that its generator $\hat{C}(\xi)$ can be defined via the action of $\hat{U}_d$ for infinitesimal diffeomorphisms d. Then it follows that Eq. (5.1) implies that $\hat{C}(\xi)$ satisfies the commutation relations implied by (2.6), that Eq. (5.2) implies that $\hat{C}(\xi)$ is self-adjoint, and that Eqs. (5.3), (5.4), and (5.5) imply that $\hat{C}(\xi)$ satisfies the commutation relations implied by Eqs. (2.8), (2.9), and (2.10). It is in this sense that Eqs. (5.1), (5.2), (5.3), (5.4), and (5.5) provide a representation of the relevant Poisson bracket algebra and "reality" conditions.

The above discussion was predicated on the assumed existence and properties of $\mathcal{G}(\mathcal{E})$. It is beyond the scope of this paper to analyze the validity of this assumption. From the discussion in [13] it seems unlikely that $\mathcal{G}(\mathcal{E})$ has the structure of an infinite dimensional group (although the situation of $1 + 1$ dimensions is probably an exception due to the existence of the infinite dimensional group of conformal isometries). It turns out that in order to apply the technique of group averaging, we need the label "d" to

take values in some group which acts on $\mathcal{E}$. In this regard, we note that the set of bijective maps from $\mathcal{E}$ to itself has the structure of a group (recall that the set of bijective maps of any set defines the symmetric group of that set [14]). We denote this group by $\mathcal{S}(\mathcal{E})$.

As we shall see, the analysis in the rest of this work holds if we replace the (putative) group $\mathcal{G}(\mathcal{E})$ by $\mathcal{S}(\mathcal{E})$. We denote the action of $d \in \mathcal{S}(\mathcal{E})$ on $X^A(x) \in \mathcal{E}$ by $X_d^A(x)$, which is a *bijective* mapping. Let $d_1 \circ d_2 \in \mathcal{S}(\mathcal{E})$ denote the map obtained by the composition of the map $d_2 \in \mathcal{S}(\mathcal{E})$ with $d_1 \in \mathcal{S}(\mathcal{E})$, i.e. $d_1 \circ d_2(X^A(x)) = d_1(X_{d_2}^A(x)) =: X_{d_1 \circ d_2}^A(x)$. As before, we define $(\phi_d(x), \pi_d(x))$ as the free field evolution of $(\phi(x), \pi(x))$ from $X^A(x)$ to $X_d^A(x)$. If $\mathcal{G}(\mathcal{E})$ with the assumed properties does not exist, the discussion in this section up to this point serves merely to motivate the imposition of Eqs. (5.1), (5.2), (5.3), (5.4), and (5.5), with d now taking values in $\mathcal{S}(\mathcal{E})$.

To summarize, we replace the set of quantum operators $\hat{H}_G, \hat{X}^A(x), \hat{\phi}(x), \hat{\pi}(x)$ by the set $\hat{U}_d, \hat{X}^A(x), \hat{\phi}(x), \hat{\pi}(x)$. If our assumption on $\mathcal{G}(\mathcal{E})$ is correct then d takes values in $\mathcal{G}(\mathcal{E})$. If $\mathcal{G}(\mathcal{E})$ (with the assumed properties) does not exist, d takes values in $\mathcal{S}(\mathcal{E})$. In either case, we impose the relations (5.1), (5.2), (5.3), (5.4), and (5.5) in addition to the commutation relations between (and the reality conditions on) the set $\hat{X}^A(x), \hat{\phi}(x), \hat{\pi}(x)$.

The imposition of these conditions, in conjunction with the demand that physical states be invariant under the action of $\hat{U}_d$, constitute our definition of the Dirac quantization of PFT.

B. $\mathcal{G}(\mathcal{E})$ versus $\mathcal{S}(\mathcal{E})$

Clearly, the replacement of $\mathcal{G}(\mathcal{E})$ by $\mathcal{S}(\mathcal{E})$ is a very nontrivial step. The group structure of $\mathcal{S}(\mathcal{E})$ has very little to do with the manifold structure of the spacetime M. This can be seen through the following example. Consider two distinct spacelike embeddings $F_1^A(x), F_2^A(x)$. Let the bijective map d be such that (i) it maps $F_1^A(x), F_2^A(x)$ to the distinct spacelike embeddings $F_{1d}^A(x), F_{2d}^A(x)$, (ii) it maps $F_{1d}^A(x)$ and $F_{2d}^A(x)$ to $F_1^A(x)$ and $F_2^A(x)$, respectively, and (iii) it is the identity on the rest of $\mathcal{E}$. We can choose $F_1^A(x)$ and $F_2^A(x)$ to define intersecting hypersurfaces in M. Since d only needs to be a bijection, we can choose $F_{1d}^A(x)$, $F_{2d}^A(x)$ such that they define nonintersecting hypersurfaces in M. Thus elements of $\mathcal{S}(\mathcal{E})$ can have a very "discontinuous" action on $\mathcal{E}$. (An even "worse" scenario is if $F_1^A(x)$ and $F_2^A(x)$ are chosen so as to define the same hypersurface in M (albeit with different coordinatizations), and $F_{1d}^A(x)$, $F_{2d}^A(x)$ are chosen such that they define distinct (say, nonintersecting) hypersurfaces in M.)

Thus, intuitively speaking, $\mathcal{S}(\mathcal{E})$ corresponds to a huge enlargement of the set of gauge transformations generated by the constraints in classical PFT. The justification for using $\mathcal{S}(\mathcal{E})$ in the quantization of PFT is an *a posteriori* one—as we shall show in Sec. VI C, the resultant quanti-

zation of PFT is equivalent to the standard Fock quantization of the free scalar field on flat spacetime. This equivalence relies on the fact that $\mathcal{S}(\mathcal{E})$ has a transitive action on $\mathcal{E}$.

In view of the above discussion, it would be desirable to replace $\mathcal{S}(\mathcal{E})$ with some subgroup thereof which is sensitive to (at least some aspects of) the manifold structure of M and which has a transitive action on $\mathcal{E}$.[10] This could be attempted by defining a topology on $\mathcal{E}$ which takes into account properties of M and by restricting attention to continuous bijections (with continuous inverses) on $\mathcal{E}$ which have a transitive action on $\mathcal{E}$. We leave such an investigation for future work.

C. Representation of $\hat{U}_d$

We define the action of $\hat{U}_d$ by its action on the embedding-dependent Fock basis states of the subspace $|F\rangle \otimes \mathcal{H}_F \subset \mathcal{H}_{\text{kin}}$ (see Eq. (4.20)). For a fixed embedding $F^A(x)$ such a Fock basis consists of the vacuum $|F\rangle \otimes |0, F\rangle$ and the "N-particle" states, $|F\rangle \otimes \prod_i^m (b_F^\dagger(\vec{k}_i))^{n_i} |0, F\rangle$. Here $N = \sum_{i=1}^m n_i$, and the N-particle states contain n_i excitations of momentum $\vec{k}_i, i = 1, \ldots, m$. The action of $\hat{U}_d$ is defined as

$$\hat{U}_d |F\rangle \otimes |0, F\rangle = |F_{d^{-1}}\rangle \otimes |0, F_{d^{-1}}\rangle, \qquad (5.6)$$

$$\hat{U}_d |F\rangle \otimes \prod_i^m (b_F^\dagger)^{n_i} |0, F\rangle = |F_{d^{-1}}\rangle \otimes \prod_i^m (b_{F_{d^{-1}}}^\dagger)^{n_i} |0, F_{d^{-1}}\rangle, \qquad (5.7)$$

embedding $F_{d^{-1}}$, obtained by the action of the above basis states. The action of $\hat{U}_d$ can be extended to any state in $|F\rangle \otimes \mathcal{H}_F$ (and then to any state in $\mathcal{H}_{\text{kin}}$) by linearity.

Next, we show that this action satisfies Eqs. (5.1), (5.2), (5.3), (5.4), and (5.5). It suffices to check the action of $\hat{U}_d$ on the vacuum and N-particle basis states defined above.

Verification of Eq. (5.1)—Recall that the notation "$F_{d^{-1}}$" in Eq. (5.12) signifies the embedding $F_{d^{-1}}$, obtained by the action of d^{-1} on the embedding $F^A(x)$. Consider the action of d_1 on $\mathcal{E}$, followed by the action of d_2 on $\mathcal{E}$. As in Eq. (5.1), we denote the resultant map on $\mathcal{E}$ by $d_2 \circ d_1$. Under this map X^A is mapped to $X_{d_1}^A$ and then to coordinates $X_{d_2 \circ d_1}^A$. Thus, we have that

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[10]$\mathcal{G}(\mathcal{E})$ with its assumed properties would be a candidate if it also had a transitive action; however, as mentioned earlier, we suspect that $\mathcal{G}(\mathcal{E})$ with the assumed properties does not exist in spacetime dimensions greater than 2.

$$\hat{U}_{d_2}\hat{U}_{d_1}|F\rangle \otimes \prod_i^m (b_F^\dagger)^{n_i}|0, F\rangle = \hat{U}_{d_2}|F_{d_1^{-1}}\rangle$$

$$\otimes \prod_i^m (b_{F_{d_1^{-1}}}^\dagger)^{n_i}|0, F_{d_1^{-1}}\rangle \tag{5.8}$$

$$= |F_{d_2^{-1}\circ d_1^{-1}}\rangle \otimes \prod_i^m (b_{F_{d_2^{-1}\circ d_1^{-1}}}^\dagger)^{n_i}|0, F_{d_2^{-1}\circ d_1^{-1}}\rangle \tag{5.9}$$

$$= |F_{(d_1\circ d_2)^{-1}}\rangle \otimes \prod_i^m (b_{F_{(d_1\circ d_2)^{-1}}}^\dagger)^{n_i}|0, F_{(d_1\circ d_2)^{-1}}\rangle \tag{5.10}$$

$$= \hat{U}_{d_1\circ d_2}|F\rangle \otimes \prod_i^m (b_F^\dagger)^{n_i}|0, F\rangle. \tag{5.11}$$

Similar considerations hold when we replace the N-particle state by the vacuum state $|0, F\rangle$ in the above equations. This completes the verification of (5.1).

While Eqs. (5.8), (5.9), (5.10), and (5.11) are straightforward to check, the notation is a bit cumbersome. It is more convenient to use the following notation instead. Given a state $|\psi, F\rangle \in \mathcal{H}_F$, we denote the action of $\hat{U}_d$ on the state $|F\rangle \otimes |\psi, F\rangle$ (obtained by the expansion of $|\psi, F\rangle \in \mathcal{H}_F$ in the Fock basis and the employment of Eqs. (5.6) and (5.7) on the basis states) by

$$\hat{U}_d|F\rangle \otimes |\psi, F\rangle =: |F_{d^{-1}}\rangle \otimes |\psi, F_{d^{-1}}\rangle. \tag{5.12}$$

In this notation we can directly verify (5.1) for any state $|F\rangle \otimes |\psi, F\rangle$ as follows:

$$\hat{U}_{d_2}\hat{U}_{d_1}|F\rangle \otimes |\psi, F\rangle = \hat{U}_{d_2}|F_{d_1^{-1}}\rangle \otimes |\psi, F_{d_1^{-1}}\rangle \tag{5.13}$$

$$= |F_{d_2^{-1}\circ d_1^{-1}}\rangle \otimes |\psi, F_{d_2^{-1}\circ d_1^{-1}}\rangle \tag{5.14}$$

$$= |F_{(d_1\circ d_2)^{-1}}\rangle \otimes |\psi, F_{(d_1\circ d_2)^{-1}}\rangle \tag{5.15}$$

$$= \hat{U}_{d_1\circ d_2}|F\rangle \otimes |\psi, F\rangle. \tag{5.16}$$

Verification of Eq. (5.2)—Consider the states $|F_1\rangle \otimes |\psi_1, F_1\rangle$, $|F_2\rangle \otimes |\psi_2, F_2\rangle$ where $|\psi_1, F_1\rangle \in \mathcal{H}_{F_1}$ and $|\psi_2, F_2\rangle \in \mathcal{H}_{F_2}$ and $F_1^A(x)$, $F_2^A(x)$ are embeddings. Recall that (,) denotes the inner product on $\mathcal{H}_{\rm kin}$ (see (4.22)). For any d we have that

$$(\hat{U}_d|F_1\rangle \otimes |\psi_1, F_1\rangle, \hat{U}_d|F_2\rangle \otimes |\psi_2, F_2\rangle)$$

$$= (|(F_1)_{d^{-1}}\rangle \otimes |\psi_1, (F_1)_{d^{-1}}\rangle, |(F_2)_{d^{-1}}\rangle \otimes |\psi_2, (F_2)_{d^{-1}}\rangle). \tag{5.17}$$

Clearly $(F_1)_{d^{-1}}^A(x) = (F_2)_{d^{-1}}^A(x)$ if $F_1^A(x) = F_2^A(x)$. Also, it is straightforward to see, from (5.6) and (5.7) in conjunction with our notation, Eq. (5.12), that for any pair of states $|\psi, F\rangle$, $|\phi, F\rangle \in \mathcal{H}_F$ and any d, the following identity holds

$$\langle\psi, F|\phi, F\rangle = \langle\psi, F_{d^{-1}}|\phi, F_{d^{-1}}\rangle. \tag{5.18}$$

It then follows from (5.17) that

$$(\hat{U}_d|F_1\rangle \otimes |\psi_1, F_1\rangle, \hat{U}_d|F_2\rangle \otimes |\psi_2, F_2\rangle)$$

$$= 0 \text{ if there exists } A, x \text{ such that } F_1^A(x) \neq F_2^A(x),$$

$$= \langle\psi_1, F_1|\psi_2, F_2\rangle \text{ if } F_1^A(x) = F_2^A(x) \quad \forall\, x, A. \tag{5.19}$$

It follows from the above equation that $\hat{U}_d$ is unitary. This, in conjunction with (5.1) yields (5.2).

Verification of Eq. (5.3)—We have that

$$\hat{U}_d\hat{X}^A(x)\hat{U}_d^\dagger|F\rangle \otimes |\psi, F\rangle = \hat{U}_d\hat{X}^A(x)|F_d\rangle \otimes |\psi, F_d\rangle \tag{5.20}$$

$$= F_d^A(x)\hat{U}_d|F_d\rangle \otimes |\psi, F_d\rangle \tag{5.21}$$

$$= \hat{X}_d^A(x)|F\rangle \otimes |\psi, F\rangle. \tag{5.22}$$

We have used (4.23) and the definition of $\hat{X}_d^A(x)$ (see the discussion following (5.5)) in the second and third lines. Note that the second and third lines themselves may be used as a precise definition of $\hat{X}_d^A(x)$, especially for the case when $d \in \mathcal{S}(\mathcal{E})$. This completes the verification of Eq. (5.3).

Verification of Eqs. (5.4) *and* (5.5)—It is more convenient to show that $\hat{U}_d$ generates the correct evolution on the operators $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$ defined via Eqs. (4.1) and (4.2) in Sec. IV A. Recall from Eq. (4.13) in Sec. IV C that the classical counterparts of $(\hat{a}_S(\vec{k}), \hat{a}_S^\dagger(\vec{k}))$ are $(a(\vec{k}), a^*(\vec{k}))$. We shall refer to the classical correspondent of the action of $\hat{U}_d$ as "the finite action of the constraints" even when $d \in \mathcal{S}(\mathcal{E})$. In this language, we have that the classical correspondent of the action of $\hat{U}_d$ on $(\hat{a}_S(\vec{k}), \hat{a}_S^\dagger(\vec{k}))$ is given by the corresponding finite action of the constraints on $(a(\vec{k}), a^*(\vec{k}))$. From the discussion in Sec. V A, it follows that this action corresponds to classical evolution from the slice $X^A(x)$ to the slice $X_d^A(x)$ where $X^A(x)$ is the embedding part of the PFT phase space data. Thus in the language and notation of free scalar field evolution employed in Sec. IV C, the modes $a(\vec{k})$, $a^*(\vec{k})$ are to be thought of as data on the slice $X^A(x)$ and hence are denoted by $\vec{a}(X)$. Then the finite action of the constraints, labeled by d, on the data $\vec{a}(X)$ is to evolve them to the data $\vec{a}(X_d)$ by scalar field evolution from the slice $X^A(x)$ to the slice $X_d^A(x)$. Thus, in the notation of Sec. IV C (see, for example, Eq. (4.17)), we have that

$$\vec{a}(X_d) = C(X_d, X)\vec{a}(X). \tag{5.23}$$

If $\hat{U}_d$ does indeed generate the correct transformations in quantum theory, then it follows that the quantum correspondent of the above equation is

$$\hat{U}_d\vec{\hat{a}}_S\hat{U}_d^\dagger = C(\hat{X}_d, \hat{X})\vec{\hat{a}}_S. \tag{5.24}$$

Here, the embedding-dependent linear transformation $C(\hat{X}_d, \hat{X})$ is obtained by replacing $X^A(x)$, $X_d^A(x)$ in $C(X_d, X)$ by $\hat{X}^A(x)$, $\hat{X}_d^A(x)$ where we have defined $\hat{X}_d^A(x)$ in Sec. VA (see the discussion following Eq. (5.5)) and through Eqs. (5.21) and (5.22). We shall now verify Eq. (5.24).

We have that

$$\hat{U}_d \vec{\hat{a}}_S \hat{U}_d^\dagger |F\rangle \otimes |\psi, F\rangle = \hat{U}_d \vec{\hat{a}}_S |F_d\rangle \otimes |\psi, F_d\rangle. \quad (5.25)$$

Using Eq. (4.19), we have that $\vec{\hat{a}}_S = C(F_d, F_0)\vec{\hat{b}}(F_d)$. Using this we obtain

$$\hat{U}_d \vec{\hat{a}}_S \hat{U}_d^\dagger |F\rangle \otimes |\psi, F\rangle = C(F_d, F_0)\hat{U}_d|F_d\rangle \otimes \vec{\hat{b}}(F_d)|\psi, F_d\rangle \tag{5.26}$$

$$= C(F_d, F_0)|F\rangle \otimes \vec{\hat{b}}(F)|\psi, F\rangle \tag{5.27}$$

$$= C(F_d, F_0)C(F_0, F)\vec{\hat{a}}_S|F\rangle \otimes |\psi, F\rangle \tag{5.28}$$

$$= C(F_d, F)\vec{\hat{a}}_S|F\rangle \otimes |\psi, F\rangle \tag{5.29}$$

$$= C(\hat{X}_d, \hat{X})\vec{\hat{a}}_S|F\rangle \otimes |\psi, F\rangle. \tag{5.30}$$

Here we have used (4.19) in (5.28) and (4.18) in (5.29). We have also used the easily verifiable fact (see the remarks at the end of Sec. IV C) that $\hat{X}^A(x)$ commutes with $\vec{\hat{a}}_S$. This completes our discussion of Eqs. (5.4) and (5.5).

To summarize, we have verified that $\mathcal{H}_{\text{kin}}$ provides a Hilbert space representation for Eqs. (4.26), (4.27), (4.28), (5.1), (5.2), (5.3), and (5.24). This implies that we have defined a ∗-representation for the set of operators $(\hat{U}_d, \hat{X}^A(x), \hat{a}_S(\vec{k}), \hat{a}_S^\dagger(\vec{k}))$ (or, equivalently, using Eqs. (4.1) and (4.2), of the set $(\hat{U}_d, \hat{X}^A(x), \hat{\phi}(x), \hat{\pi}(x))$). We now proceed to an implementation of Dirac quantization along the lines employed in LQG [8].

VI. DIRAC QUANTIZATION

Just as in the case of the spatial diffeomorphism constraints in LQG, $\hat{U}_d$ does not have the appropriate continuity in d to allow a definition of its (putative) generator $\hat{C}_A(x)$. Clearly, this is so for $d \in \mathcal{G}(\mathcal{E})$ and is expected to be so for $d \in \mathcal{S}(\mathcal{E})$ for any reasonable topology on $\mathcal{S}(\mathcal{E})$. If $\hat{C}_A(x)$ is not defined, the identification of its kernel as the space of physical states is not possible. In such a case we can still use the LQG method of group averaging [8,9] to construct the physical state space. After some preliminary remarks in Sec. VI A, we discuss the construction of the physical Hilbert space $\mathcal{H}_{\text{phys}}$ in Sec. VI B and the action of Dirac observables on physical states in Sec. VI C. We shall see that the resultant quantization is equivalent to the standard Fock space quantization. In Sec. VI D we show how to obtain the action of $\hat{C}_A(x)$ on physical states as

functional Schrödinger equations in the case when operator evolution is unitary and all the embedding-dependent Hilbert spaces $\{\mathcal{H}_F\}$ are identical. We shall attempt a reasonably self-contained exposition. However the reader is urged to consult Refs. [8,9] for details regarding the group averaging technique. We shall intersperse our exposition with remarks pertaining to the analogy with structures in LQG. These remarks may be ignored by readers unfamiliar with LQG.

A. Preliminary remarks

(i) Given $F_1^A(x), F_2^A(x) \in \mathcal{E}$, $\mathcal{H}_{F_1}$ can be identified with $\mathcal{H}_{F_2}$ by an identification of the Fock basis states as follows. Identify $|0, F_1\rangle$ with $|0, F_2\rangle$ and identify the N-particle states (see Sec. V C) $\prod_i^m (b_{F_1}^\dagger(\vec{k}_i))^{n_i}|0, F_1\rangle$ with $\prod_i^m (b_{F_2}^\dagger(\vec{k}_i))^{n_i}|0, F_2\rangle$. Since any state can be expanded in the above Fock basis, every state in $\mathcal{H}_{F_1}$ has a counterpart in $\mathcal{H}_{F_2}$ and vice versa. We shall use the notation $|\psi, F_1\rangle$ and $|\psi, F_2\rangle$ to denote the states so identified. Clearly, if $F_1^A(x) = F_{2d}^A(x)$ for some (not necessarily unique) choice of d, we have that

$$|F_2\rangle \otimes |\psi, F_2\rangle := \hat{U}_d|F_1\rangle \otimes |\psi, F_1\rangle, \tag{6.1}$$

which is consistent with the notation of Eq. (5.12).

(ii) Note that even if $d \in \mathcal{G}(\mathcal{E})$, d defines a bijective map on $\mathcal{E}$. This follows from the fact that $\forall F^A(x) \in \mathcal{E}$, there exists $\bar{F}^A(x) = F_{d^{-1}}^A(x) \in \mathcal{E}$ so that $F^A(x) = \bar{F}_d^A(x)$.

(iii) Let $\mathcal{D}^*$ denote the vector space of complex linear mappings from $\mathcal{D} \subset \mathcal{H}_{\text{kin}}$ (see Eq. (4.21)) to the set of complex numbers. $\mathcal{D}^*$ is called the *algebraic dual* to $\mathcal{D}$. Elements of $\mathcal{D}^*$ are called *distributions*. Consider any operator $\hat{A}$ on $\mathcal{H}_{\text{kin}}$ such that $\hat{A}^\dagger$ maps $\mathcal{D}$ into itself. Define the action of $\hat{A}$ on $\mathcal{D}^*$ as follows. Let $\boldsymbol{\Psi} \in \mathcal{D}^*$ map $|\phi\rangle \in \mathcal{D}$ to the complex number $\boldsymbol{\Psi}(|\phi\rangle)$. Define $\hat{A}\boldsymbol{\Psi}$ by

$$\hat{A}\boldsymbol{\Psi}(|\phi\rangle) := \boldsymbol{\Psi}(\hat{A}^\dagger|\phi\rangle). \tag{6.2}$$

Let $\hat{A}, \hat{B}$ be operators such that the operators $\hat{A}^\dagger, \hat{B}^\dagger, \hat{A}^\dagger\hat{B}^\dagger, \hat{B}^\dagger\hat{A}^\dagger$ map $\mathcal{D}$ into itself. Then we have that

$$\hat{A}\hat{B}\,\boldsymbol{\Psi}(|\phi\rangle) = \hat{B}\boldsymbol{\Psi}(\hat{A}^\dagger|\phi\rangle) = \boldsymbol{\Psi}(\hat{B}^\dagger\hat{A}^\dagger|\phi\rangle), \tag{6.3}$$

so that the action of the commutator $[\hat{A}, \hat{B}]$ on $\boldsymbol{\Psi}$ is

$$[\hat{A}, \hat{B}]\boldsymbol{\Psi}(|\phi\rangle) = \boldsymbol{\Psi}([\hat{B}^\dagger, \hat{A}^\dagger]|\phi\rangle) = \boldsymbol{\Psi}([\hat{A}, \hat{B}]^\dagger|\phi\rangle). \tag{6.4}$$

Equation (6.4) implies that $\mathcal{D}^*$ provides an antirepresentation for the operators $\hat{A}, \hat{B}$.

B. Physical states through group averaging

For the remainder of this work, we shall restrict attention to the case that $d \in \mathcal{S}(\mathcal{E})$. Our considerations will also apply unchanged if $\mathcal{G}(\mathcal{E})$ is such that given $F_1^A(x), F_2^A(x) \in$

$\mathcal{E}$, there exists $d \in \mathcal{G}(\mathcal{E})$ such that $F^A_{1d}(x) = F^A_2(x)$. If $\mathcal{G}(\mathcal{E})$ does not have this property there may be superselection sectors in the physical state space constructed via group averaging. Since we do not even know if $\mathcal{G}(\mathcal{E})$ exists, much less the structure of $\mathcal{G}(\mathcal{E})$, we leave the analysis for this case for future work.

1. Construction of the space of physical states

Physical states must be invariant under the action of $\hat{U}_d$, i.e. $\Psi \in \mathcal{H}_{\text{phys}}$ if $\forall \ d$, $\hat{U}_d \Psi = \Psi$. We can formally construct such a state as follows. Define Ψ by the formal sum

$$\Psi = \sum_{F \in \mathcal{E}} |F\rangle \otimes |\psi, F\rangle. \tag{6.5}$$

Here, we have used the notation defined in (i) above. Then we have that

$$\hat{U}_d \Psi = \hat{U}_d \sum_{F \in \mathcal{E}} |F\rangle \otimes |\psi, F\rangle \tag{6.6}$$

$$= \sum_{F_{d^{-1}} \in \mathcal{E}} |F_{d^{-1}}\rangle \otimes |\psi, F_{d^{-1}}\rangle \tag{6.7}$$

$$= \sum_{F \in \mathcal{E}} |F\rangle \otimes |\psi, F\rangle = \Psi. \tag{6.8}$$

The formal sum in (6.5), in the language of group averaging, corresponds to the choice of a discrete measure on $\mathcal{S}(\mathcal{E})$. To see this, we note that we can define

$$\Psi = \left(\sum_{d \in \mathcal{S}(\mathcal{E})} \hat{U}_d\right)|F_1\rangle \otimes |\psi, F_1\rangle, \tag{6.9}$$

where $F^A_1(x)$ is some fixed embedding and the discrete measure on $\mathcal{S}(\mathcal{E})$ is such that the right-hand sides of (6.5) and (6.9) are identical. Note that $F^A_1(x)$ has a nontrivial "isotropy group" [8], i.e. the subgroup of $\mathcal{S}(\mathcal{E})$ which leaves $F^A_1(x)$ invariant. The sum in Eq. (6.9) is, therefore, not over the entire group $\mathcal{S}(\mathcal{E})$, but only over the orbit of the state $|F_1\rangle \otimes |\psi, F_1\rangle$.

The sum (6.5) is a formal one. To make our considerations well defined, it is appropriate to think of Ψ as defining the distribution $\Psi \in \mathcal{D}^*$ through

$$\Psi = \sum_{F \in \mathcal{E}} \langle \psi, F| \otimes \langle F|. \tag{6.10}$$

The sum in (6.10) is to be interpreted through the action of Ψ on $\mathcal{D}$ as follows. Ψ maps the state $|F_1\rangle \otimes |\phi, F_1\rangle$ to the complex number $\Psi(|F_1\rangle \otimes |\phi, F_1\rangle)$, where

$$\Psi(|F_1\rangle \otimes |\phi, F_1\rangle) = \left(\sum_{F \in \mathcal{E}} |F\rangle \otimes |\psi, F\rangle, |F_1\rangle \otimes |\phi, F_1\rangle\right) \tag{6.11}$$

$$= \sum_{F \in \mathcal{E}} \delta_{F,F_1} \langle \psi, F_1 | \phi, F_1\rangle \tag{6.12}$$

$$= \langle \psi, F_1 | \phi, F_1\rangle, \tag{6.13}$$

where we have used the definition (see Eq. (4.22)) of the inner product on $\mathcal{H}_{\text{kin}}$ in the second line.

The action of Ψ can be extended to all of $\mathcal{D}$ by linearity. The invariance of Ψ (6.8) translates to the easily verifiable statement that $\forall \ |\phi\rangle \in \mathcal{D}$,

$$\hat{U}_d \Psi(|\phi\rangle) = \Psi(\hat{U}^\dagger_d |\phi\rangle) = \Psi(|\phi\rangle). \tag{6.14}$$

From (6.9) it follows that Ψ can also be defined by

$$\Psi = \sum_d \langle \psi, F_1| \otimes \langle F_1 | \hat{U}^\dagger_d, \tag{6.15}$$

where the sum over d is again to be interpreted as a sum over the orbit of the state $|F_1\rangle \otimes |\psi, F_1\rangle$ rather than over the entire group $\mathcal{S}(\mathcal{E})$. Since the sum in (6.9) and (6.15) is over elements of (a (nonunique) subset of) the group $\mathcal{S}(\mathcal{E})$, this technique of constructing physical states from kinematic ones is called group averaging.

We denote the finite linear span of the set of invariant distributions (i.e. those defined through Eq. (6.10) for all choices of $|\psi, F\rangle$) by $\mathcal{D}^*_{\text{phys}}$. Thus $\Phi \in \mathcal{D}^*_{\text{phys}}$ if $\Phi = \sum^N_{I=1} c_I \Phi_I$, with c_I being complex numbers and each Φ_I being of the form (6.10),

$$\Phi_I = \sum_{F \in \mathcal{E}} \langle \phi_I, F| \otimes \langle F|. \tag{6.16}$$

We shall see that $\mathcal{D}^*_{\text{phys}}$ can be equipped with a natural inner product thus converting it into the Hilbert space $\mathcal{H}_{\text{phys}}$. Before introducing this inner product, it is useful to understand the structure of $\mathcal{D}^*_{\text{phys}}$ better. We do this by defining the group averaging map η [8].

2. The group averaging map η

Equation (6.15) defines a map from states of the form $|F\rangle \otimes |\psi, F\rangle$ to states in $\mathcal{D}^*_{\text{phys}}$. This map can be extended to all of $\mathcal{D}$ by antilinearity. In the notation of Ref. [8], this map is denoted by η. Explicitly, $\eta: \mathcal{D} \to \mathcal{D}^*_{\text{phys}}$ is defined as follows. Let $|\phi\rangle \in \mathcal{D}$ so that

$$|\phi\rangle = \sum^N_{I=1} a_I |F_I\rangle \otimes |\phi_I, F_I\rangle. \tag{6.17}$$

Then $\eta|\phi\rangle =: \Phi$ is given by the following expression:

$$\Phi = \sum^N_{I=1} a^*_I \left(\sum_d \langle \phi_I, F_I| \otimes \langle F_I | \hat{U}^\dagger_d\right) = \sum^N_{I=1} a^*_I \Phi_I \tag{6.18}$$

with $\Phi_I = \sum_{F \in \mathcal{E}} \langle \phi_I, F| \otimes \langle F|$.

From the definition of $\mathcal{D}^*_{\text{phys}}$, it follows that the antilinear map η is onto. The map η has a nontrivial kernel. This can be seen as follows. The action of Φ defined in Eq. (6.18) on any state $|\psi\rangle \in \mathcal{D}$,

$$|\psi\rangle := \sum_{J=1}^{M} b_J |G_J\rangle \otimes |\psi_J, G_J\rangle \qquad (6.19)$$

is

$$\Phi(|\psi\rangle) = \sum_{I=1}^{N} \sum_{J=1}^{M} a_I^* b_J \langle \phi_I, G_J |\psi_J, G_J\rangle. \qquad (6.20)$$

From Eq. (6.1) and the fact that $\hat{U}_d$ is unitary, it follows that $\Phi(|\psi\rangle)$ can also be written as

$$\Phi(|\psi\rangle) = \sum_{I=1}^{N} \sum_{J=1}^{M} a_I^* b_J \langle \phi_I, F |\psi_J, F\rangle, \qquad (6.21)$$

for any $F^A(x) \in \mathcal{E}$. This implies that $\Phi(|\psi\rangle) = 0 \; \forall \; |\psi\rangle \in \mathcal{D}$ if $\forall F^A(x) \in \mathcal{E}$,

$$\sum_{I=1}^{N} a_I^* \langle \phi_I, F| \otimes \langle F| = 0. \qquad (6.22)$$

Equation (6.22) implies that the kernel of η consists of all $|\phi\rangle \in \mathcal{D}$, $|\phi\rangle = \sum_{I=1}^{N} a_I F_I \otimes |\phi_I, F_I\rangle \in \mathcal{D}$ with a_I, $|\phi_I, F_I\rangle$ such that Eq. (6.22) holds.

The above structure of the kernel implies that every element of $\mathcal{D}_{\text{phys}}^*$ is of the form (6.10). More precisely, let Φ be an arbitrary element of $\mathcal{D}_{\text{phys}}^*$. Then, as can be verified, there exists a unique state $|\phi, F\rangle \in \mathcal{H}_F$ such that $\forall \; F^A(x) \in \mathcal{E}$,

$$\Phi = \eta|F\rangle \otimes |\phi, F\rangle. \qquad (6.23)$$

3. The inner product on $\mathcal{D}_{\text{phys}}^*$

The map η endows $\mathcal{D}_{\text{phys}}^*$ with the following inner product. Let $\Psi, \Phi \in \mathcal{D}_{\text{phys}}^*$. Then their inner product is defined as

$$(\Psi, \Phi) = \Phi(|\psi\rangle), \qquad (6.24)$$

where $|\psi\rangle \in \mathcal{D}$ is any state in $\mathcal{D}$ such that $\eta|\psi\rangle = \Psi$.

We note the following:

(a) The right-hand side of Eq. (6.24) is independent of the choice of $|\psi\rangle$: Let $|\psi_1\rangle, |\psi_2\rangle$ be such that $\eta|\psi_1\rangle = \eta|\psi_2\rangle = \Psi$. Then $|\psi_1\rangle - |\psi_2\rangle$ is in the kernel of η. From Eq. (6.22) this means that $|\psi_1\rangle - |\psi_2\rangle = \sum_{J=1}^{M} b_J |G_J\rangle \otimes |\psi_J, G_J\rangle$ with b_J, $|\psi_J, G_J\rangle$ such that

$$\sum_{J=1}^{M} b_J^* \langle \psi_J, F| \otimes \langle F| = 0, \quad \forall \; F^A(x) \in \mathcal{E}. \qquad (6.25)$$

Let $\Phi = \eta|\phi\rangle$ with $|\phi\rangle \in \mathcal{D}$ given by $|\phi\rangle = \sum_{I=1}^{N} a_I |F_I\rangle \otimes |\phi_I, F_I\rangle$. Then $\Phi(|\psi_1\rangle - |\psi_2\rangle)$ is given by Eq. (6.21), the right-hand side of which vanishes as a result of Eq. (6.25). Thus $\Phi(|\psi_1\rangle) = \Phi(|\psi_2\rangle)$.

(b) The inner product is Hermitian: Let $\Phi, |\psi\rangle$ be given by Eqs. (6.18) and (6.19) with a_I, b_J not necessarily satisfying Eqs. (6.22) and (6.25). Then from Eq. (6.21),

we have that

$$(\Psi, \Phi) = (\Phi(|\psi\rangle)) = \sum_{I=1}^{N} \sum_{J=1}^{M} a_I^* b_J \langle \phi_I, F |\psi_J, F\rangle$$

$$= (\Phi, \Psi)^*. \qquad (6.26)$$

(c) Equation (6.24) is linear in its second element and antilinear in its first element. This follows from the linear vector space structure of $\mathcal{D}_{\text{phys}}^*$ and the antilinearity of the map η.

(d) The inner product is positive definite: Let $\Phi = \eta|\phi\rangle$ be given by Eqs. (6.17) and (6.18) with a_I not necessarily satisfying Eq. (6.22). Then

$$(\Phi, \Phi) = \Phi(|\phi\rangle) = \sum_{I=1}^{N} \sum_{J=1}^{N} a_I^* a_J \langle \phi_I, F |\phi_J, F\rangle$$

$$= \langle \phi, F |\phi, F\rangle \qquad (6.27)$$

with $|\phi, F\rangle = \sum_{I=1}^{N} a_I |\phi_I, F\rangle$. Thus $(\Phi, \Phi) \geq 0$ and vanishes only if $|\phi, F\rangle = 0$, i.e. only if $|\phi\rangle$ is in the kernel of η (see Eq. (6.22)).

(e) As in Footnote 6, we shall gloss over mathematical niceties related to the distinction between operators and operator valued distributions, as well as issues related to unbounded operators and dense domains. However, we do note here that the completion of the space $\mathcal{D}_{\text{phys}}^*$ in the inner product (6.24) does not enlarge $\mathcal{D}_{\text{phys}}^*$ so that, as vector spaces, $\mathcal{D}_{\text{phys}}^* = \mathcal{H}_{\text{phys}}$. The interested reader may easily verify this fact by using Eq. (6.23) and noting that $\mathcal{H}_F, F^A(x) \in \mathcal{E}$ are Hilbert spaces and hence Cauchy complete.

C. Dirac observables
1. Classical theory

From the work of Kuchař [1,2] it follows that Dirac observables can be identified with the values of the phase space variables $(\phi(x), \pi(x))$, or equivalently, $\vec{a}(X)$ (see the discussion before Eq. (5.23) for the definition of $\vec{a}(X)$) at some initial embedding, say $F_0^A(x)$. We denote the Dirac observables corresponding to the values of $\vec{a}(X)$ at $F_0^A(x)$ by $\vec{a}_D = a_D(\vec{k}), a_D^*(\vec{k})$. Thus $\vec{a}_D$ is given by the expression

$$\vec{a}_D := C(F_0, X)\vec{a}(X). \qquad (6.28)$$

The following argument shows that $a_D(\vec{k}), a_D^*(\vec{k})$ are indeed Dirac observables. Consider a finite transformation generated by the constraints which evolves the data $(X^A(x), \vec{a}(X))$ to $(X_d^A(x), \vec{a}(X_d))$. Denote $\vec{a}_D$ evaluated on the new data by $(\vec{a}_D)_d$. Then we have that

$$\begin{aligned} (\vec{a}_D)_d &= C(F_0, X_d)\vec{a}(X_d) \\ &= C(F_0, X_d)C(X_d, X)\vec{a}(X) \\ &= C(F_0, X)\vec{a}(X) = \vec{a}_D, \end{aligned} \qquad (6.29)$$

where we used Eqs. (4.17) and (4.18) in the second line. Thus $a_D(\vec{k})$, $a_D^*(\vec{k})$ are invariant under the action of the constraints. Hence they are classical Dirac observables.

Clearly, since $\vec{a}_D$ is related to $\vec{a}(X)$ via a canonical transformation only dependent on $X^A(x)$, it follows that the Poisson brackets between $a_D(\vec{k})$, $a_D^*(\vec{k})$ are given by

$$\{a_D(\vec{k}), a_D(\vec{l})\} = 0 = \{a_D^*(\vec{k}), a_D^*(\vec{l})\},$$
$$\{a_D(\vec{k}), a_D^*(\vec{l})\} = i\delta(\vec{k}, \vec{l}). \qquad (6.30)$$

2. Quantum theory

The quantum correspondent of Eq. (6.28) is

$$\hat{\vec{a}}_D := C(F_0, \hat{X})\hat{\vec{a}}_S, \qquad (6.31)$$

where $C(F_0, \hat{X})$ is defined by replacing $X^A(x)$ by $\hat{X}^A(x)$ in the expression for $C(F_0, X)$. The action of $\hat{\vec{a}}_D$ on $|F\rangle \otimes |\psi, F\rangle$ is given by

$$\hat{\vec{a}}_D|F\rangle \otimes |\psi, F\rangle = C(F_0, \hat{X})\hat{\vec{a}}_S|F\rangle \otimes |\psi, F\rangle \qquad (6.32)$$

$$= C(F_0, F)\hat{\vec{a}}_S|F\rangle \otimes |\psi, F\rangle \qquad (6.33)$$

$$= C(F_0, F)C(F, F_0)|F\rangle \otimes \vec{b}(F)|\psi, F\rangle \qquad (6.34)$$

$$= \vec{b}(F)|F\rangle \otimes |\psi, F\rangle. \qquad (6.35)$$

We have used the fact that $\hat{X}^A(x)$ commutes with $\hat{\vec{a}}_S$ (see Eq. (4.26) in (6.33). Equation (6.33) follows from the definition of $\hat{\vec{a}}_S$ in Eq. (4.19). Equation (6.35) implies that $\hat{\vec{a}}_D$ has the following properties.

(a) $\hat{\vec{a}}_D$ maps physical states to physical states: Let $\boldsymbol{\Phi} \in \mathcal{D}_{\text{phys}}^*$. Then it follows from Eq. (6.23) that $\boldsymbol{\Phi}$ is of the form $\boldsymbol{\Phi} = \eta|\phi\rangle$, $|\phi\rangle = |F\rangle \otimes |\phi, F\rangle$. Let $|\psi\rangle \in \mathcal{D}$, $|\psi\rangle = |G\rangle \otimes |\psi, G\rangle$. Then

$$\hat{a}_D(\vec{k})\boldsymbol{\Phi}(|\psi\rangle) = \boldsymbol{\Phi}(\hat{a}_D^\dagger(\vec{k})|\psi\rangle) \qquad (6.36)$$

$$= \boldsymbol{\Phi}(|G\rangle \otimes \hat{b}_G^\dagger(\vec{k})|\psi\rangle) \qquad (6.37)$$

$$= \langle\phi, G|\hat{b}_G^\dagger(\vec{k})|\psi, G\rangle \qquad (6.38)$$

$$=: \boldsymbol{\Phi}_{\hat{a}_D(\vec{k})}(|\psi\rangle), \qquad (6.39)$$

where

$$\boldsymbol{\Phi}_{\hat{a}_D(\vec{k})} = \eta(\hat{b}_F(\vec{k})|F\rangle \otimes |\phi, F\rangle). \qquad (6.40)$$

Since states of the form $|G\rangle \otimes |\psi, G\rangle$ are a basis for $\mathcal{D}$, and since $\eta(\hat{b}_F(\vec{k})|\phi\rangle)$ is independent of the choice of $F^A(x) \in \mathcal{E}$, it follows that $\hat{a}_D(\vec{k})\boldsymbol{\Phi}$ is of the form (6.10) and is hence a physical state. Similar considerations hold for $\hat{a}_D(\vec{k})^\dagger$.

(b) The action of the operators $\hat{a}_D(\vec{k})$, $\hat{a}_D^\dagger(\vec{k})$ on physical states provides an anti-representation of their Poisson bracket relations (6.30): Given $\boldsymbol{\Phi} \in \mathcal{D}_{\text{phys}}^*$ and $|\psi\rangle = |F\rangle \otimes |\psi, F\rangle$, we have that

$$(\hat{a}_D(\vec{k})\hat{a}_D^\dagger(\vec{l})\boldsymbol{\Phi})(|\psi\rangle) = (\hat{a}_D^\dagger(\vec{l})\boldsymbol{\Phi})(|F\rangle \otimes \hat{b}_F^\dagger(\vec{k})|\psi, F\rangle) \qquad (6.41)$$

$$= \boldsymbol{\Phi}(|F\rangle \otimes \hat{b}_F(\vec{l})\hat{b}_F^\dagger(\vec{k})|\psi, F\rangle), \qquad (6.42)$$

so that $[\hat{a}_D(\vec{k})\hat{a}_D(\vec{l})^\dagger] = [\hat{b}_F(\vec{l}), \hat{b}_F^\dagger(\vec{k})] = \delta(\vec{k}, \vec{l})$. Similar calculations, with the same choice of $|\psi\rangle$ as in the above equations show that the commutators $[\hat{a}_D(\vec{k}), \hat{a}_D(\vec{l})]$, $[\hat{a}_D^\dagger(\vec{k}), \hat{a}_D^\dagger(\vec{l})]$ are mapped to the commutators $[\hat{b}_F^\dagger(\vec{l}), \hat{b}_F^\dagger(\vec{k})]$, $[\hat{b}_F(\vec{l}), \hat{b}_F(\vec{k})]$. Note that (i) $\hat{b}_F(\vec{k})$, $\hat{b}_F^\dagger(\vec{k})$ are annihilation, creation operators on $\mathcal{H}_F$, (ii) Eq. (6.42) (and similar equations for the other commutators) is independent of the choice of $F^A(x)$, and (iii) states of the form $|F\rangle \otimes |\psi, F\rangle$, $F^A(x) \in \mathcal{E}$ provide a basis for $\mathcal{D}$.

It follows from (i)–(iii) that Eq. (6.35) defines an anti-representation, on $\mathcal{H}_{\text{phys}}$, of the Poisson algebra generated by the Poisson brackets (6.30).

(c) The operators $\hat{a}_D(\vec{k})$, $\hat{a}_D^\dagger(\vec{k})$ are adjoint to each other on $\mathcal{H}_{\text{phys}}$: Let $\boldsymbol{\Psi}_i = \eta|\psi_i\rangle$, $|\psi_i\rangle = |F\rangle \otimes |\psi_i, F\rangle$, $i = 1, 2$ (Eq. (6.23) implies that this choice of $|\psi_i\rangle$ involves no loss of generality). Then we have that

$$(\boldsymbol{\Psi}_1, \hat{a}_D(\vec{k})\boldsymbol{\Psi}_2)) = \boldsymbol{\Psi}_2(\hat{b}_F^\dagger(\vec{k})|F\rangle \otimes |\psi_1, F\rangle) \qquad (6.43)$$

$$= \langle\psi_2, F|\hat{b}_F^\dagger(\vec{k})|\psi_1, F\rangle, \qquad (6.44)$$

$$(\boldsymbol{\Psi}_2, \hat{a}_D^\dagger(\vec{k})\boldsymbol{\Psi}_1)) = \boldsymbol{\Psi}_1(\hat{b}_F(\vec{k})|F\rangle \otimes |\psi_2, F\rangle) \qquad (6.45)$$

$$= \langle\psi_1, F|\hat{b}_F(\vec{k})|\psi_2, F\rangle. \qquad (6.46)$$

Since $\hat{b}_F(\vec{k})$', $\hat{b}_F^\dagger(\vec{k})$ are Hermitian conjugates on $\mathcal{H}_F$, it follows that $(\boldsymbol{\Psi}_1, \hat{a}_D(\vec{k})\boldsymbol{\Psi}_2))^* = (\boldsymbol{\Psi}_2, \hat{a}_D^\dagger(\vec{k})\boldsymbol{\Psi}_1))$ thus implying that $(\hat{a}_D(\vec{k}))^\dagger = \hat{a}_D^\dagger(\vec{k})$ on $\mathcal{H}_{\text{phys}}$.

3. Equivalence with the standard Fock representation

Recall that in the standard Fock quantization, the field operator $\hat{\phi}(X)$ is given by the expression

$$\hat{\phi}(X) = \frac{1}{(2\pi)^{n/2}} \int \frac{d^n k}{\sqrt{2k}} (\hat{\mathbf{a}}(\vec{k})e^{-ikT+i\vec{k}\cdot\vec{X}}$$
$$+ \hat{\mathbf{a}}^\dagger(\vec{k})e^{ikT-i\vec{k}\cdot\vec{X}}), \qquad (6.47)$$

where we have used the notation $X^0 = T$ and $\{X^A, A = 1, \ldots, n\} = \vec{X}$. The operators $\hat{\mathbf{a}}(\vec{k})$, $\hat{\mathbf{a}}^\dagger(\vec{k})$ are the annihilation and creation operators on the standard Fock space $\mathcal{F}$. The standard Fock vacuum is denoted by $|0\rangle$ so that $\hat{\mathbf{a}}(\vec{k})|0\rangle = 0 \; \forall \; \vec{k}$ and $\mathcal{F}$ is generated by the (repeated)

action of the creation operators $\hat{\mathbf{a}}^\dagger(\vec{k})$ on $|0\rangle$. We denote the pair $\hat{\mathbf{a}}(\vec{k})$, $\hat{\mathbf{a}}^\dagger(\vec{k})$ by $\vec{\hat{\mathbf{a}}}$.[11]

We shall now show that this quantization is equivalent to the Dirac quantization of PFT constructed in this work. We proceed in two steps. First we show that $|F_0\rangle \otimes \mathcal{H}_{F_0}$ is naturally isomorphic to $\mathcal{H}_{\text{phys}}$. Next we show that $|F_0\rangle \otimes \mathcal{H}_{F_0}$ is also naturally isomorphic to $\mathcal{F}$ and that the consequent isomorphism between $\mathcal{F}$ and $\mathcal{H}_{\text{phys}}$ renders the two representations equivalent.

Equations (6.22) and (6.23) imply that η restricted to $|F_0\rangle \otimes \mathcal{H}_{F_0}$ is bijective. Specifically, (6.22) and (6.23) imply that every $|\psi\rangle \in |F_0\rangle \otimes \mathcal{H}_{F_0}$ is uniquely mapped to $\Psi \in \mathcal{H}_{\text{phys}}$ via $\eta|\psi\rangle = \Psi$. Further, given $|\psi\rangle, |\phi\rangle \in |F_0\rangle \otimes \mathcal{H}_{F_0}$, we have that

$$(\eta|\psi\rangle, \eta|\phi\rangle) = \langle\phi|\psi\rangle, \tag{6.48}$$

$$\hat{a}_D(\vec{k})\eta|\phi\rangle = \eta\hat{b}_{F_0}(\vec{k})|\phi\rangle, \tag{6.49}$$

$$\hat{a}_D^\dagger(\vec{k})\eta|\phi\rangle = \eta\hat{b}_{F_0}^\dagger(\vec{k})|\phi\rangle. \tag{6.50}$$

These equations imply that η defines a 1-1, antilinear map from $|F_0\rangle \otimes \mathcal{H}_{F_0}$ to $\mathcal{H}_{\text{phys}}$ which induces an antilinear $\star$-homomorphism from the $\star$-algebra of operators generated by $\hat{b}_{F_0}(\vec{k})$, $\hat{b}_{F_0}^\dagger(\vec{k})$ to that generated by $\hat{a}_D(\vec{k})$, $\hat{a}_D^\dagger(\vec{k})$.[12]

Next, note that the representation of the $\star$-algebra of operators generated by $\hat{b}_{F_0}(\vec{k})$, $\hat{b}_{F_0}^\dagger(\vec{k})$ on $|F_0\rangle \otimes \mathcal{H}_{F_0}$ is (trivially) unitarily related to that generated by $\hat{\mathbf{a}}(\vec{k})$, $\hat{\mathbf{a}}^\dagger$ on $\mathcal{F}$. Explicitly, we define this relation via the map $U: \mathcal{F} \rightarrow |F_0\rangle \otimes \mathcal{H}_{F_0}$ where

$$U|0\rangle = |F_0\rangle \otimes |0, F_0\rangle, \tag{6.51}$$

$$U\prod_i^m (\hat{\mathbf{a}}^\dagger(\vec{k}_i))^{n_i}|0\rangle = \prod_i^m (\hat{b}_{F_0}^\dagger(\vec{k}_i))^{n_i}|F_0\rangle \otimes |0, F_0\rangle. \tag{6.52}$$

Clearly, we have that[13]

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[11]In the notation employed in Sec. IV B, the operators $\vec{\hat{\mathbf{a}}}$ would be denoted by $\vec{\hat{a}}_H(F_0)$ since they are the Heisenberg picture representatives of the classical variables $\vec{a}(X)$ on the initial slice $X^A(x) = F_0^A(x)$. This notation (and a suitable notation for the individual annihilation and creation operators) is cumbersome and this is why we have used the simpler notation with the bold face.

[12]The operators which generate the algebra are related by adjointness relations. These relations induce adjointness relations among elements of the algebra in the obvious way. Such an algebra with adjointness relations is called a $\star$-algebra. A $\star$-homomorphism between two $\star$-algebras preserves both the algebraic and the adjointness relations between elements of the algebras. For a more precise definition of these structures, see, for example, Ref. [8].

[13]Equation (4.19) implies that $\vec{\hat{b}}(F_0) = \vec{\hat{a}}_S$. The discussion in Secs. IV B and IV C suggests that $\hat{a}_S$ be associated with the "time zero" Heisenberg operators $\vec{\hat{a}}_H(F_0)$. The discussion after (6.47) with regard to notation implies this association is consistent with Eq. (6.53) below.

$$U\vec{\hat{\mathbf{a}}}U^\dagger = \vec{\hat{b}}(F_0). \tag{6.53}$$

It follows that the map $\mathcal{U} := \eta \circ U$ is a 1-1, antilinear map from $\mathcal{F}$ to $\mathcal{H}_{\text{phys}}$ which induces an antilinear $\star$-homomorphism from the $\star$-algebra of operators generated by $\hat{\mathbf{a}}(\vec{k})$, $\hat{\mathbf{a}}^\dagger(\vec{k})$ to that generated by $\hat{a}_D(\vec{k})$, $\hat{a}_D^\dagger(\vec{k})$. In language shorn of mathematical jargon, all we are saying is that the Dirac quantization constructed here is unitarily equivalent to the conjugate representation defined by the Fock representation, where, by conjugate representation we mean the representation defined on "bra" states from that defined by "ket" states. This completes our proof of the physical equivalence of the standard Fock quantization and the Dirac quantization described in this paper.

D. The functional Schrödinger equation in $1 + 1$ dimensions

In this section, our aim is to reveal the structures in the Dirac quantization of PFT which allow for the possibility of defining functional Schrödinger equations in $1 + 1$ dimensions of the type considered in Refs. [3,4]. We shall assume familiarity with the contents and results of Refs. [3,4] and limit our exposition to a rephrasing of those results in terms of the structures defined here.

We start with a few remarks which lead to a caveat regarding the applicability of the Torre-Varadarajan analysis to the case of noncompact Cauchy slices considered here. Torre and Varadarajan [4] showed that in $1 + 1$ dimensions, free scalar field evolution from an initial flat slice to an arbitrary slice of flat spacetime is unitarily implemented in the standard Fock space quantization. They defined Schrödinger picture states by the action of the inverse (embedding-dependent) unitary transformation on (embedding-independent) states in the standard Fock space. By functionally differentiating the Schrödinger picture states with respect to the embedding, TV showed that these states satisfy a functional Schrödinger equation which corresponds to a rigorous definition of Eq. (1.2) in quantum theory. This rigorously defined Schrödinger equation was anticipated in full detail by Kuchař in [3]; in terms of structures introduced in [3,4]. The TV results in $1 + 1$ dimensions [4] were derived for compact Cauchy slices diffeomorphic to the circle. In this paper, for the case of $1 + 1$ dimensions, we have considered noncompact Cauchy slices diffeomorphic to the real line. Hence, strictly speaking, the TV results do not apply here. However, TV have persuasively argued in Sec. V of Ref. [4] that their results should also apply to the case of the spatial topology being that of the line.[14] Therefore we shall simply assume that the relevant TV structures exist in the case of the noncompact Cauchy slices considered here.

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[14]Conversely, we believe that our general considerations here should apply with suitable modifications to the case of compact Cauchy slices.

It is beyond the scope of this paper to provide a detailed generalization of the TV analysis to the noncompact case. We now proceed to a rephrasing of the (assumed) TV results in terms of our constructions in this work.

Note that if evolution between $F_0^A(x)$ and any $F^A(x) \in \mathcal{E}$ is unitary on $\mathcal{F}$, it follows that all the Hilbert spaces $\mathcal{H}_F$, $F^A(x) \in \mathcal{E}$ are identical. We denote this single Schrödinger picture Hilbert space by $\mathcal{H}$. Of course $\mathcal{H} = \mathcal{F}$; we use a different notation only to remind the reader that we are dealing with a Schrödinger picture representation.

Next, note that if $\hat{P}_A(x)$ was a well-defined operator on $\mathcal{H}_{\mathrm{kin}}$, we could directly evaluate its action on $\boldsymbol{\Psi} \in \mathcal{H}_{\mathrm{phys}}$ via the dual action (6.2). However, as mentioned earlier, besides the problems described in Sec. V, the operator $\hat{H}_G$ does not have the requisite continuity in $G^A(x)$ to define $\hat{P}_A(x)$. Specifically, the limit

$$\lim_{\epsilon \to 0} \frac{\hat{H}_{\epsilon G} - 1}{i\epsilon} |\psi\rangle := \int dx \, G^A(x) \hat{P}_A(x) |\psi\rangle \qquad (6.54)$$

for $|\psi\rangle \in \mathcal{D}_X$ does not exist on the Hilbert space $\mathcal{H}_X$ (see Sec. III C for a discussion of $\mathcal{D}_X$, $\mathcal{H}_X$). Although this limit does not exist on $\mathcal{H}_X$, we show below that such a limit can be defined on a suitable subspace of the algebraic dual space $\mathcal{D}^*$ (see (iii) of Sec. VI A for the definition of $\mathcal{D}^*$).

Let $\boldsymbol{\Psi} = \sum_{\bar{F} \in \mathcal{E}} \langle \psi, \bar{F}| \otimes \langle \bar{F}| \in \mathcal{H}_{\mathrm{phys}}$. We define the "partial" action of $\boldsymbol{\Psi}$ on $|F\rangle$, $F^A(x) \in \mathcal{E}$ as follows:

$$\boldsymbol{\Psi}(|F\rangle) := \left(\sum_{\bar{F} \in \mathcal{E}} |\bar{F}\rangle \otimes |\psi, \bar{F}\rangle, |F\rangle \right) \qquad (6.55)$$

$$= \sum_{\bar{F} \in \mathcal{E}} \delta_{\bar{F}, F} \langle \psi, \bar{F}| \qquad (6.56)$$

$$= \langle \psi, F|. \qquad (6.57)$$

Next, consider the action on $\boldsymbol{\Psi}$, of the operator $\frac{\hat{H}_{\epsilon G} - 1}{i\epsilon}$, in the context of this partial action. We have that

$$\left(\frac{\hat{H}_{\epsilon G} - 1}{i\epsilon} \boldsymbol{\Psi} \right)(|F\rangle) = \boldsymbol{\Psi}\left(\frac{\hat{H}_{\epsilon G}^\dagger - 1}{-i\epsilon} |F\rangle \right) \qquad (6.58)$$

$$= \boldsymbol{\Psi}\left(\frac{|F + \epsilon G\rangle - |F\rangle}{-i\epsilon} \right) \qquad (6.59)$$

$$= \frac{\langle \psi, F + \epsilon G| - \langle \psi, F|}{-i\epsilon}. \qquad (6.60)$$

Note that in general $F^A(x) + \epsilon G^A(x) \notin \mathcal{E}$ for arbitrary $F^A(x)$, $G^A(x)$, ϵ. However, for a given $G^A(x)$ of compact support and $F^A(x) \in \mathcal{E}$, it is straightforward to see that there exists $\epsilon_0 > 0$ such that $\forall\ \epsilon$ satisfying the condition $0 < \epsilon < \epsilon_0$, we have that $F^A(x) + \epsilon G^A(x) \in \mathcal{E}$.[15] Thus,

Eq. (6.60) is well defined for sufficiently small ϵ. Note that such an equation would not be meaningful if $\mathcal{H}_{F + \epsilon G}$ and $\mathcal{H}_F$ were not identical. This is expected to happen in higher dimensions for generic choices of $F^A(x)$, $G^A(x)$ [5]. Thus Eq. (6.60) is expected to only make sense in $1 + 1$ dimensions or in the context of special choices of $F^A(x)$, $G^A(x)$ in higher dimensions.

The $\epsilon \to 0$ limit of Eq. (6.60) exists on the Hilbert space $\mathcal{H}$ provided $|\psi, F + \epsilon G\rangle$ is sufficiently well behaved in ϵ. If this happens we may write the $\epsilon \to 0$ limit of (6.60) as

$$\lim_{\epsilon \to 0}\left(\frac{\hat{H}_{\epsilon G} - 1}{i\epsilon} \boldsymbol{\Psi} \right)(|F\rangle) = i \int dx \, G^A(x) \frac{\delta}{\delta F^A(x)} \langle \psi, F|. \qquad (6.61)$$

As we argue below such well-behavedness should follow from a specification of the Schrödinger picture-vacuum state along the lines of Ref. [4]. Recall that we defined $|0, F\rangle$ to be the state annihilated by the operators $\hat{b}_F(\vec{k})$, $\forall\ \vec{k}$. This definition only specifies $|0, F\rangle$ up to an $F^A(x)$ dependent phase. For an arbitrary choice of this phase, the $\epsilon \to 0$ limit of Eq. (6.60) may not exist.

In [4], the embedding-dependent-Schrödinger picture vacuum is constructed by the action of the exponential of an operator, quadratic in the creation operators, on the standard Fock vacuum, multiplied by an explicitly defined embedding-dependent normalization factor. The coefficients of the creation operators in the exponent are constructed out of the Bogoliubov coefficients which define the classical canonical transformation corresponding to (inverse) evolution from the embedding back to the initial flat slice. These structures are in correspondence with the following structures in this work. Clearly the creation operators correspond to $\mathbf{a}^\dagger(\vec{k})$ and the standard Fock vacuum to $|0\rangle$. Footnote 12, together with the fact that $\mathcal{H} = \mathcal{F}$, implies the identifications $\hat{b}_{F_0}^\dagger(\vec{k}) = \hat{a}_S^\dagger(\vec{k}) = \mathbf{a}^\dagger(\vec{k})$ and $|0, F_0\rangle = |0\rangle$ (in fact, we fix the phase ambiguity in the definition of $|0, F_0\rangle$ by this identification). The Bogoliubov transformation is $C(F, F_0)$ and the Bogoliubov coefficients are $\alpha_{F, F_0}(\vec{k}, \vec{l})$, $\beta_{F, F_0}(\vec{k}, \vec{l})$ where $\vec{k}, \vec{l}$ are in correspondence with the set of real numbers since they are spatial vectors in 1 dimension (see Eq. (4.16) for the definition of α, β).

We expect that, as in the spatially compact case, the Schrödinger picture vacuum can be explicitly constructed along the lines of [4] and that, as in [4], it is functionally differentiable with respect to the embedding. Thus, we expect that Eq. (6.61) is well defined for $|\psi, F\rangle = |0, F\rangle$. The Schrödinger picture N-particle states of Sec. V C can then be obtained by the repeated action of the creation operators $\hat{b}_F^\dagger(\vec{k})$ on $|0, F\rangle$. From [4] we expect that these states should also be functionally differentiable with respect to $F^A(x)$. It follows that any $|\psi, F\rangle$ which is a suitably well-behaved linear combination of these basis states is also functionally differentiable. The right-hand side of Eq. (6.61) can be explicitly computed for such states in

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[15]We expect that a similar result should be true for $G^A(x)$, $F^A(x)$ satisfying suitable "asymptotically flat" conditions which allow for more general $G^A(x)$.

terms of the functional derivatives of the basis states. We expect that the latter can be computed along the lines of [4] and that here, in close analogy to the result of such a computation in Ref. [4], $\langle \psi, F|$ satisfies a rigorously defined functional Schrödinger equation with a precisely defined, nontrivial operator ordering prescription for $\hat{h}_A(x)$ and an additional c-number correction.[16]

This completes our discussion of the (expected) derivation of the $1 + 1$-dimensional functional Schrödinger equation from the Dirac quantization constructed in this paper.

VII. DISCUSSION

In particle quantum mechanics, the Heisenberg picture is identified with the Schrödinger picture at some initial instant of time. In the case of $n + 1$-dimensional PFT, Torre and Varadarajan choose this identification to be at an initial flat slice defined by $X^A(x) = (0, x^1, \ldots, x^n)$. Their results imply that embedding-dependent Schrödinger picture states cannot be constructed as the unitary images of (embedding-independent) states in the standard (Heisenberg picture) Fock space, $\mathcal{F}$, for generic choices of embedding and for $n > 1$. This rules out the possibility of defining (unitary) functional evolution of states on $\mathcal{F}$.[17]

While such evolution of states in the single Hilbert space $\mathcal{F}$ is ruled out, TV showed that functional evolution of states *can* be defined, provided the notion of a quantum state is enlarged to that used in algebraic quantum field theory [5]. There, algebraic states are identified with PLFs on the Weyl algebra (see, for example, [12]). Conversely, every PLF on the Weyl algebra defines, through the Gelfand-Naimark-Segal (GNS) construction [12], a Hilbert space representation of the Weyl algebra. This representation is such that there is a state in the GNS Hilbert space for which the expectation value of any Weyl algebra element is the same as the evaluation of the PLF on this element. Consider the Weyl algebra for a free scalar field on flat spacetime. Inverse evolution from any embedding to the initial flat embedding is a canonical transformation and, hence, defines an automorphism of the Weyl algebra [5]. The induced action of this automorphism on any PLF defines a new PLF, i.e. a new algebraic state. Any state in $\mathcal{F}$ defines, via its expectation values in the standard Fock representation, a PLF on the Weyl algebra. The action of the automorphism corresponding

to inverse evolution from an arbitrary embedding to the initial flat one on this PLF yields an embedding-dependent PLF, i.e. an embedding-dependent algebraic state. It is in this sense that functional evolution of algebraic states is well defined.

In the context of this algebraic quantum field theory viewpoint, the TV results indicate that the GNS Hilbert space representation associated with a generic embedding is inequivalent to the Fock space representation. Indeed, the embedding-dependent Hilbert spaces $\mathcal{H}_F$ defined in Sec. IV D are precisely the embedding-dependent GNS Hilbert spaces.[18] Thus, our work can be considered to be an implementation, using LQG techniques, of algebraic state evolution in the context of the single, nonseparable Hilbert space $\mathcal{H}_{\text{kin}}$ (4.20). Moreover, even though generic scalar field evolution is not unitary on $\mathcal{F}$, the evolution generated by the constraints, as defined by $\hat{U}_d$, *is* unitary on the "much larger" Hilbert space $\mathcal{H}_{\text{kin}}$ (see Sec. V B). Clearly, the LQG type of representation of the embedding variables plays a key role in this unitarity.

Despite our demonstration that the TV results are not an obstruction to a Dirac quantization of PFT, these results *can* be restated in the context of Dirac quantization as follows. Rather than interpret them in the context of a (putative) Schrödinger picture, the TV results can be interpreted within the context of Heisenberg picture-based quantizations. In this context, they imply the existence of inequivalent quantizations of the free scalar field. These arise from inequivalent complex structures, i.e. inequivalent choices of basic annihilation and creation operators. Specifically, given an embedding $F_1^A(x)$, the operators $\vec{\hat{\mathbf{a}}}_1 = C(F_0, F_1)\vec{\hat{\mathbf{a}}}$ (see Eq. (6.47) for the definition of $\vec{\hat{\mathbf{a}}}$) are the annihilation and creation operators for the Hilbert space $\mathcal{H}_{F_1}$. Any embedding-dependent Heisenberg picture operator can be constructed from the operators corresponding to $\vec{\hat{\mathbf{a}}}$, and then reexpressed in terms of the operators $\vec{\hat{\mathbf{a}}}_1$. If the Bogoliubov transformation $C(F_0, F_1)$ is not unitarily implementable on $\mathcal{F}$ then the Heisenberg picture representation on $\mathcal{H}_{F_1}$ is inequivalent to the standard Heisenberg picture Fock representation on $\mathcal{F}$. This unitary inequivalence can be traced to the fact that the operator $\hat{N}_0$ which measures the number of excitations associated with $\vec{\hat{\mathbf{a}}}$ (i.e. $\hat{N}_0 = \int d^n k \hat{\mathbf{a}}^\dagger(\vec{k})\hat{\mathbf{a}}(\vec{k})$) has a well-defined vacuum expectation value in $\mathcal{F}$ but not in $\mathcal{H}_{F_1}$ (where the vacuum state in $\mathcal{H}_{F_1}$ is defined to be $|0, F_1\rangle$) [12]. Conversely the number operator $\hat{N}_1$ for the excitations associated with the operators $\vec{\hat{\mathbf{a}}}_1$ has a well-defined vacuum expectation value in $\mathcal{H}_{F_1}$ but not in $\mathcal{F}$.

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[16]The expected functional Schrödinger equation may be identified with a definition of the constraint operator $\hat{C}_A(x)$ on $\mathcal{H}$. As in Refs. [3,4], the c-number correction is expected to compensate for a Virasoro type anomaly in the constraint algebra which arises if $\hat{C}_A(x)$ is defined without this additional correction; it is only with this correction that the constraint algebra is expected to close [3].

[17]Since embeddings are specified by functions-worth of data, we refer to the evolution from the initial slice to an arbitrary final one as "functional" evolution.

[18]Denote the GNS Hilbert space associated with $F^A(x)$ by $\mathcal{H}_F^{(\text{GNS})}$. Then $\mathcal{H}_F^{(\text{GNS})}$ is naturally identified with $\mathcal{H}_F$ in such a way that $\hat{\mathbf{a}}(\vec{k})$, $\hat{\mathbf{a}}^\dagger(\vec{k})$ are mapped to $\hat{a}_S(\vec{k})$, $\hat{a}_S^\dagger(\vec{k})$. See Footnote 13 with regard to the naturalness of this identification.

A Dirac quantization of PFT, equivalent to this quantization, can be constructed by replacing the operators $\vec{\hat{b}}(F)$ by (in obvious notation) the operators $\vec{\hat{h}}(F) = C(F_0, F_1)\vec{\hat{b}}(F)$,[19] and the Dirac observables $\vec{\hat{a}}_D$ by the Dirac observables $\vec{\hat{a}}_{(1)D} = C(F_0, F_1)\hat{a}_D$, in our constructions. Thus, the new kinematic Hilbert space, $\mathcal{H}^1_{\mathrm{kin}}$, is given by $\mathcal{H}^1_{\mathrm{kin}} = \bigoplus_F |F\rangle \otimes \mathcal{H}^1_F$ where $\mathcal{H}^1_F$ is the Fock space associated with the annhilation and creation operators $\hat{h}(\vec{k})$, $\hat{h}^\dagger(\vec{k})$. The interested reader can check that all the steps go through and one obtains a quantization equivalent to the Heisenberg picture quantization on $\mathcal{H}_{F_1}$. In this quantization the Dirac observable $\hat{N}_{(0)D} = \int d^n k \hat{a}^\dagger_D(\vec{k})\hat{a}_D(\vec{k})$ does not have a well-defined vacuum expectation value (where the vacuum is defined to be the state annihilated by $\hat{a}_{(1)D}(\vec{k})$) whereas the Dirac observable $\hat{N}_{(1)D} = \int d^n k \hat{a}^\dagger_{(1)D}(\vec{k})\hat{a}_{(1)D}(\vec{k})$ does have a well-defined (vanishing) vacuum expectation value. Conversely $\hat{N}_{(1)D}$ does not have a well-defined vacuum expectation value in the representation constructed in Sec. VI (where the vacuum is defined to be the state annihilated by $\hat{a}_D(\vec{k})$) whereas the vacuum expectation value of $\hat{N}_{(0)D}$ vanishes. This concludes our discussion of the relation of the TV results to the constructions of this work.

We shall discuss the very interesting open issue regarding the existence and structure of $\mathcal{G}(\mathcal{E})$ towards the end of this section. Now, we turn to a summary of technical details which need to be worked out in the Dirac quantization of PFT. As mentioned in Sec. II B, we have not specified asymptotic boundary conditions on the embedding variables. As mentioned in Footnote 6, we have been cavalier about the distinctions between genuine operators and operator valued distributions, as well as those between bounded and unbounded operators. We feel that these details can easily be supplied in a more careful treatment and that our results will be unaffected. In Sec. VI D, we assumed that our results would also apply, in the $1 + 1$-dimensional case, to spatially compact slices of topology S^1. In the spatially compact case, there are two new ingredients. The first is the absence of global inertial coordinates. This should easily be handled, as in [2], by describing the embedding variables as suitable maps from S^1 to the spacetime. The second new ingredient is the appearance of "zero modes" of the scalar field; these are quantum *mechanical* (as opposed to field theoretic) degrees of freedom and we expect that they can be accommodated without changing our basic results, but this needs to be worked out. Note also that, in the case studied in this work (i.e. the case of the spatial topology being that of R^n), we have not explicitly worked out the Bogoliubov coef-

ficients. As noted in [4], there may be infrared problems when $n = 1$—we refer the reader to the comments in [4] as they apply here as well. Note that in this case (i.e. of the spatial topology being that of a line), a Dirac quantization of PFT different from ours, has been recently constructed by Laddha [15]. It would be of interest to compare his quantization with ours.

Let us assume that our results do go through as envisaged in $1 + 1$ dimensions for the spatially compact case. Then Footnote 16 indicates that despite an anomaly free quantization of the constraints, the formalism is still sensitive to the Virasoro anomaly. Further, as stressed by Kuchař in [3], although there is no anomaly in the algebra of constraints due to the compensating "anomaly potential" term, there *is* the usual Virasoro anomaly in the algebra of Dirac observables which correspond to the normal ordered stress-energy fluxes. Since the closed bosonic string can be realized as a PFT with an additional constraint [11], we believe that a Dirac quantization, along the lines sketched here, of this system should be possible and should yield a quantization identical to that of [11]. It would be of interest to attempt to construct such a quantization and compare it with Thiemann's quantization of the string [16].

We also believe that our constructions here can be suitably (and trivially) modified so as to apply to the case of axisymmetric PFT in $2 + 1$ dimensions. Thus, we expect that despite the results of [6], it is possible to construct a Dirac quantization of the system which is equivalent to the standard Fock quantization. The results of [5,6] obtained in the context of higher dimensional PFTs and cylindrical waves seemed to raise apprehensions about the physical viability of any Dirac quantization based approach to quantum gravity. It is ironical that in the light of our results here, the Dirac quantization of these systems (certainly PFTs and most likely, cylindrical waves, in their reformulation as axisymmetric PFTs) are beautiful examples of the power of the techniques developed in one such approach, namely, that of LQG.

As mentioned earlier in this section, we shall now turn to a discussion of the most interesting open issue in this work, namely, that of a precise characterization of the space of finite canonical transformations generated by the smeared constraints $C(\xi)$ of Eq. (2.7). Recall that the problem is that while the Poisson bracket algebra of the smeared constraints is isomorphic to the Lie bracket of vector fields on the spacetime, the finite canonical transformations generated by $C(\xi)$ are not in correspondence with the group of all spacetime diffeomorphisms because the latter do not leave the space of spacelike embeddings, $\mathcal{E}$, invariant. It is therefore of interest to know whether there exists an infinite dimensional space of diffeomorphisms which keep $\mathcal{E}$ invariant. If this (putative) space exists as the group $\mathcal{G}(\mathcal{E})$ of Sec. VA, and if $\mathcal{E}$ can be generated by the action of $\mathcal{G}(\mathcal{E})$ on any fixed element of $\mathcal{E}$, the technique of group averaging yields the Dirac quantization constructed in this work. If

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[19] In order not to have too cumbersome a notation, we have omitted to signify the dependence of $\hat{h}(F)$ on the fixed embedding $F_1^A(x)$.

$\mathcal{G}(\mathcal{E})$ does not have this property, we expect the existence of superselection sectors in the space of physical states. Clearly, the detailed structure of $\mathcal{G}(\mathcal{E})$ (if it exists) determines the structure of the physical Hilbert space.

Since the work of [13] seems to indicate that $\mathcal{G}(\mathcal{E})$ may not exist as an infinite dimensional group, we have replaced the set of finite canonical transformations generated by the smeared constraints by the (intuitively) much larger set of transformations labeled by bijections from $\mathcal{E}$ to itself, i.e. by elements of $\mathcal{S}(\mathcal{E})$. As discussed in Sec. V B, such bijections do not have any continuity properties reflective of the differential structure of the spacetime manifold M. Nevertheless, this ''enlargement'' of the set of gauge transformations in quantum theory yields the physically correct quantization on a *separable* Hilbert space. It would be useful to understand exactly why this happens. This enlargement of the notion of gauge is reminiscent of the proposed enlargement of the spatial diffeomorphism gauge in LQG by Zapata [17]. Zapata showed that his proposal lead to a separable Hilbert space prior to the imposition of the Hamiltonian constraint. It is not clear what repercussions Zapata's proposed enlargement of spatial diffeomorphism gauge has on the classical limit of LQG. By virtue of the close analogy between structures in the Dirac quantization of PFT and in LQG, we hope that this work may be of some use in clarifying the above issue as well as other issues (such as those of interpretation) in LQG. Note that one key difference between the PFT case and LQG is that in the former, the smeared constraints form a Lie algebra. It may be of interest to see if progress can be made in an LQG type of quantization of more complicated systems in which the constraint algebra is a Lie algebra, such as that of gravity with appropriate matter [18].

Finally, we note that in this work our aim was to provide a Dirac quantization of PFT which is unitarily equivalent to the standard Fock representation of flat spacetime free scalar field theory. We achieved this despite the TV results, by a combination of an LQG type representation for the embedding variables and Fock type representations for the scalar field variables. One may, of course, enquire as to the existence of a Dirac quantization of PFT in which both sets of variables (i.e. embedding and scalar field) are represented in LQG type representations. Although the question is open for higher dimensions, significant progress has been made by Laddha in the case of $1 + 1$ dimensions [15].

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