Functional evolution of free quantum fields

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Abstract

We consider the problem of evolving a quantum field between any two (in general, curved) Cauchy surfaces. Classically, this dynamical evolution is represented by a canonical transformation on the phase space for the field theory. We show that this canonical transformation cannot, in general, be unitarily implemented on the Fock space for free quantum fields on flat spacetimes of dimension greater than 2. We do this by considering time evolution of a free Klein-Gordon field on a flat spacetime (with toroidal Cauchy surfaces) starting from a flat initial surface and ending on a generic final surface. The associated Bogolubov transformation is computed; it does not correspond to a unitary transformation on the Fock space. This means that functional evolution of the quantum state as originally envisioned by Tomonaga, Schwinger, and Dirac is not a viable concept. Nevertheless, we demonstrate that functional evolution of the quantum state *can* be satisfactorily described using the formalism of algebraic quantum field theory. We discuss possible implications of our results for canonical quantum gravity.

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I. INTRODUCTION

In this paper we consider some aspects of dynamical evolution in quantum field theory. Specifically, we examine the description of dynamics in which one evolves the state of a quantum field from any initial Cauchy surface to any final Cauchy surface, rather than just between Cauchy surfaces of constant Minkowskian time. This way of formulating dynamical evolution dates back to the inception of relativistic quantum field theory. We begin our introduction to the main ideas via a brief historical sketch.

The idea of evolving a quantum field from any Cauchy surface to any other seems to have originated in the mid 1940's with the work of Tomonaga [1] and Schwinger [2] on relativistic quantum field theory. Tomonaga and Schwinger wanted an invariant generalization of the Schrödinger equation, which describes time evolution of the state of a quantum field relative to a fixed inertial reference frame. By allowing for all possible Cauchy surfaces in the description of dynamical evolution one easily accommodates all possible notions of time for all possible inertial observers. Thus a dynamical formalism incorporating arbitrary Cauchy surfaces does allow for an invariant generalization of the Schrödinger equation. Since, the space of Cauchy surfaces is infinite-dimensional, it is impossible to describe time evolution along arbitrary surfaces by using a single time parameter. In essence, one needs a distinct time parameter for every possible foliation of spacetime. As shown by Tomonaga and Schwinger, if one formulates dynamics in terms of general Cauchy surfaces, the resulting dynamical evolution equation is, formally, a functional differential equation, which is usually called the "Tomonaga-Schwinger equation". Following [3], we use the term *functional evolution* to refer to the formulation of dynamical evolution in which one evolves quantities along arbitrary Cauchy surfaces.[1] Thus the Tomonaga-Schwinger equation appears as the analog of the Schrödinger equation, when describing functional evolution. It was (and still is) tacitly assumed that the Tomonaga-Schwinger equation defines the infinitesimal form of unitary evolution of states from one Cauchy surface to another, just as the more familiar (and mathematically more tractable) Schrödinger equation describes the infinitesimal form of unitary evolution between two hyperplanes of constant Minkowskian time. One of our principal goals in this paper is to show that this assumption is untenable.

In the book *Lectures on Quantum Mechanics* [4], Dirac considers the problem of evolving a quantum field from any Cauchy surface to any other. He calls this the problem of "quantization on curved surfaces". He does not actually solve this problem, but rather sets up a constrained Hamiltonian field theory (sometimes called a "parametrized field theory") that allows for evolution of the classical field along any foliation of spacetime by Cauchy surfaces. He then considers the canonical quantization of this constrained Hamiltonian field theory. In this approach to functional evolution, the Tomonaga-Schwinger equation arises, formally, as the condition that constraints annihilate physical states. Dirac concludes that the principal difficulty that arises is in finding a factor-ordering of the operators representing energy and momentum densities, which are to generate the dynamical evolution, so that the

[1] Synonyms for functional evolution in the physics literature include: "many-fingered time" evolution, "hypertime" evolution, and "bubble time" evolution.

state function can be evolved consistently by the Tomonaga-Schwinger equation. This is essentially the "problem of functional evolution", discussed by Kuchař in [3]. Dirac indicates that this problem should not arise for fields that are "simple" enough, but that for field theories such as Born-Infeld electrodynamics the factor ordering problems are very severe.

As pointed out by Dirac, to obtain a description of the dynamics of a quantum field in accord with the special theory of relativity, as is appropriate for non-gravitational physics, it is not necessary to go so far as to allow for *all* Cauchy surfaces in the evolution of the quantum state. It is enough to secure a formulation of dynamics that allows for – and does not distinguish between – all notions of time defined by inertial observers. One now has only a finite number of generators to define, and a much weaker set of requirements to be put on them, namely, they must obey the Poincaré algebra. However, when considering physical theories constructed in accord with the general theory of relativity, which is mandatory when describing gravitating systems, one does not (in general) have any preferred notions of time and one is obliged to consider dynamical evolution using arbitrary Cauchy surfaces. Of course, it is a violation of the basic spirit of general relativity if one class of Cauchy surfaces is physically distinguished from another in the quantum theory. Thus, in general relativistic physics, whether one is considering quantum fields on a fixed classical spacetime or considering a quantum gravitational field, one is naturally led to use a functional evolution formalism to describe the dynamics of the quantum field.

Motivated by issues in canonical quantum gravity, Kuchař began investigating the functional evolution of a free scalar field on a flat, two-dimensional cylindrical spacetime [5]. This work was continued in [6] by the present authors. For our purposes, the principal results of [5] and [6] are as follows. (1) Dynamical evolution between any pair of smooth Cauchy surfaces (actually, curves) is consistently and unitarily implemented on the standard Fock space representation of the quantum field; and as a consequence, (2) the Tomonaga-Schwinger equation can be rigorously defined and solved for this model. It was noted in [6] that generalizations of results (1) and (2) to flat spacetimes of higher dimension do not seem to exist. Our goal in this paper is to follow up on this observation.

The extensive exploration of quantum field theory on a curved spacetime over the past 3 decades naturally has strong overlap with the investigation being reported here. The situation in a curved spacetime is, however, complicated by the fact that, for a generic spacetime, there is considerable freedom in the choice of Hilbert space representation of the canonical commutation relations (CCR) for the field. For our purposes, the most significant results can be found in the work of Helfer [7]. He considers dynamical evolution of a free field in curved spacetime with initial and final surfaces being constant time surfaces in static regions (the "in" and "out" regions) of spacetime. He shows that if one uses a Hadamard representation of the CCR then the dynamical evolution cannot be unitarily implemented. Helfer shows that the putative generators of the functional evolution (namely, spatial integrals of certain components of the quantized energy-momentum tensor) necessarily have rather pathological properties. He also points out that the difficulties with defining the quantized generators of functional evolution already occur in flat spacetime. Again, one is led to believe that difficulties with the functional evolution formalism will occur in spacetimes of dimension greater than 2, even when the spacetime is flat.

In what follows we will try to make this last statement more precise and give a "no-go" result for the functional evolution formalism for free fields on a flat spacetime of dimension greater than 2. We begin in section II by giving a formulation of the functional evolution formalism (for a Klein-Gordon field) using the framework of algebraic quantum field theory. This approach to quantum field theory has become more or less standard; it represents something of a generalization of the more traditional quantum field theory formalism, which is based upon Hilbert space, linear operators, etc. The algebraic approach is especially well-suited to functional evolution of quantum fields and, as far as we develop it here, appears to have no fundamental difficulties. The difficulties with functional evolution appear when trying to reduce the algebraic approach to the usual Hilbert space framework. In particular, in section III we show that the usual Fock space for a Klein-Gordon field on a flat spacetime with topology $\mathbf{R} \times \mathbf{T}^n$ does not allow for unitary transformations that implement functional evolution. We conclude with further discussion of this result and some comments on implications for canonical quantum gravity. Some technical details are collected in a couple of appendices.

II. ALGEBRAIC APPROACH TO FUNCTIONAL EVOLUTION

A. Classical Preliminaries

Here we consider the functional evolution of a free, classical Klein-Gordon field φ with mass m on an $(n{+}1)$-dimensional, globally hyperbolic spacetime (M, g). There is a result due to Geroch [8] that guarantees the existence of a foliation of M by spacelike Cauchy surfaces diffeomorphic to an n-dimensional manifold Σ. In other words, there is a diffeomorphism $\Psi\colon \mathbf{R}\times\Sigma \to M$, such that for each element of $\mathbf{R}$ the image of Σ is a spacelike Cauchy surface. The foliation defined by Ψ is not unique, and we aim to describe the time evolution with respect to an arbitary choice of foliation. In section III we will specialize to the case where $\Sigma = \mathbf{T}^n$ and g is flat.

The field equations are

$$(g^{ab}\nabla_a\nabla_b - m^2)\varphi = 0. \tag{2.1}$$

We let Γ denote the space of smooth solutions to (2.1) with compactly supported Cauchy data. The Cauchy data are a pair of fields (ϕ, π) on Σ, where ϕ is a scalar field and π is a scalar density of weight one. Given a solution φ to (2.1), ϕ is the pull-back of φ to Σ and π is the pull-back to Σ of the normal derivative of φ multiplied by the square root of the determinant of the induced metric on Σ. The pull-back, normal, and induced metric are determined by the embedding $T\colon \Sigma \to M$ of Σ as a Cauchy hypersurface $T(\Sigma)$ in M. The space of (smooth, compactly supported) Cauchy data will be denoted by Υ. Because the Cauchy data uniquely determine a solution, and *vice versa*, the vector spaces Γ and Υ are naturally isomorphic once one has specified a Cauchy surface $T(\Sigma)$. We denote this isomorphism by $\mathcal{I}_T$. The map $\mathcal{I}_T\colon \Upsilon \to \Gamma$ is obtained by taking Cauchy data (a point in Υ) and evolving from the Cauchy surface $T(\Sigma)$ to get a solution of (2.1) (a point of Γ). The inverse map, $\mathcal{I}_T^{-1}\colon \Gamma \to \Upsilon$, takes a solution to (2.1) and finds the Cauchy data induced on Σ by virtue of the embedding T.

Either of the spaces Γ or Υ can be viewed as the classical phase space for the Klein-Gordon field (see, e.g., [9]). In particular, the phase space in each case is naturally equipped with a symplectic form, that is, a skew-symmetric, bilinear, non-degenerate 2-form. On the space of solutions Γ, the symplectic form is defined as

$$\Omega(\varphi_1, \varphi_2) = \int_{T(\Sigma)} \sqrt{\gamma}\,(\varphi_2 L_n \varphi_1 - \varphi_1 L_n \varphi_2)\,, \tag{2.2}$$

where L_n is the Lie derivative along the normal to the Cauchy surface $T(\Sigma)$ and γ is the determinant of the induced metric on $T(\Sigma)$. The integral is evaluated on the Cauchy surface $T(\Sigma)$, but Ω is independent of the choice of $T\colon \Sigma \to M$. On the space of Cauchy data Υ, the symplectic form is defined by

$$\sigma((\phi_1, \pi_1), (\phi_2, \pi_2)) = \int_\Sigma (\phi_2 \pi_1 - \phi_1 \pi_2)\,. \tag{2.3}$$

It is easy to see that, for any embedding T, the isomorphism $\mathcal{I}_T$ is a symplectic map from Υ to Γ:

$$\sigma = \mathcal{I}_T^* \Omega. \tag{2.4}$$

We now describe time evolution on the classical phase space. We begin with evolution as represented on Υ since this setting is probably most familiar. Given initial and final Cauchy surfaces, represented by embeddings T_{I} and T_{F}, we view time evolution from $T_{\mathrm{I}}(\Sigma)$ to $T_{\mathrm{F}}(\Sigma)$ as a map $\tau_{(T_{\mathrm{I}},T_{\mathrm{F}})}\colon \Upsilon \to \Upsilon$, where

$$\tau_{(T_{\mathrm{I}},T_{\mathrm{F}})} = \mathcal{I}_{T_{\mathrm{F}}}^{-1} \circ \mathcal{I}_{T_{\mathrm{I}}}. \tag{2.5}$$

This map arises from the following 3 steps: (i) take initial data on $T_{\mathrm{I}}(\Sigma)$, (ii) evolve it to a solution of (2.1), and (iii) find the data that are induced on $T_{\mathrm{F}}(\Sigma)$ by this solution. The map $\tau_{(T_{\mathrm{I}},T_{\mathrm{F}})}$ is a bijection.

Time evolution from T_{I} to T_{F} can also be viewed as a bijection $\mathcal{T}_{(T_{\mathrm{I}},T_{\mathrm{F}})}\colon \Gamma \to \Gamma$ on the space of solutions. We define this map by

$$\mathcal{T}_{(T_{\mathrm{I}},T_{\mathrm{F}})} = \mathcal{I}_{T_{\mathrm{I}}} \circ \mathcal{I}_{T_{\mathrm{F}}}^{-1}. \tag{2.6}$$

Viewed as a map on the space of solutions to the Klein-Gordon equation, time evolution from T_{I} to T_{F} is obtained from the following 3 steps: (i) take a solution to the field equations, (ii) find the data induced on $T_{\mathrm{F}}(\Sigma)$, (iii) take that data as initial data on $T_{\mathrm{I}}(\Sigma)$ and find the resulting solution.

The relation between the maps τ and $\mathcal{T}$ is through the isomorphism $\mathcal{I}$. More precisely, if we use the initial embedding T_{I} to identify Γ and Υ, then we can use $\mathcal{I}_{T_{\mathrm{I}}}$ to carry τ from Υ to Γ. We then find

$$\mathcal{I}_{T_{\mathrm{I}}} \circ \tau_{(T_{\mathrm{I}},T_{\mathrm{F}})} \circ \mathcal{I}_{T_{\mathrm{I}}}^{-1} = \mathcal{T}_{(T_{\mathrm{I}},T_{\mathrm{F}})}. \tag{2.7}$$

The two descriptions of time evolution, using either τ or $\mathcal{T}$, are equivalent. Moreover, from the embedding independence of (2.2) and from (2.4), each is a symplectic isomorphism:

$$\tau_{(T_{\mathrm{I}},T_{\mathrm{F}})}^* \sigma = \sigma, \quad \mathcal{T}_{(T_{\mathrm{I}},T_{\mathrm{F}})}^* \Omega = \Omega. \tag{2.8}$$

This is just a field-theoretic implementation of the familiar result that "time evolution is a canonical transformation".

To summarize, the space of solutions Γ of (2.1) (or space of Cauchy data Υ for (2.1)) is a symplectic vector space. Time evolution between arbitrary Cauchy surfaces is a symplectic transformation on Γ (Υ). It is a matter of convenience whether we describe dynamics using the space of solutions or the space of Cauchy data. For the most part, we will present our discussion using Γ, Ω and $\mathcal{T}$.

B. Quantum Field Theory

A formulation of quantum field theory that readily allows for time evolution between arbitrary Cauchy surfaces is provided by the algebraic approach [10]. The main ingredients in the algebraic approach are (i) a C^* algebra $\mathcal{A}$ of basic observables and (ii) states, which are positive, normalized, linear functions $\omega\colon \mathcal{A} \to \mathbf{C}$. The value of a state ω on an observable $W \in \mathcal{A}$ is interpreted as the expectation value of the observable represented by W in the state represented by ω:

$$\langle W \rangle = \omega(W). \tag{2.9}$$

For free fields, the algebra $\mathcal{A}$ is taken to be the Weyl algebra, which is naturally available on any symplectic vector space such as Γ (or Υ) and encodes the information about the canonical commutation relations. The Weyl algebra is generated by elements $W(\varphi)$, labeled by points $\varphi \in \Gamma$, satisfying

$$W(\varphi)^* = W(-\varphi) \tag{2.10}$$

$$W(\varphi_1)W(\varphi_2) = e^{-i\Omega(\varphi_1,\varphi_2)}W(\varphi_1+\varphi_2). \tag{2.11}$$

Given two algebras $\mathcal{A}_1$ and $\mathcal{A}_2$, each with generators satisfying (2.10) and (2.11), there exists a unique $*$-isomorphism $\alpha\colon \mathcal{A}_1 \to \mathcal{A}_2$ such that for any $W_1 \in \mathcal{A}_1$ and $W_2 \in \mathcal{A}_2$, we have

$$\alpha \cdot W_1 = W_2. \tag{2.12}$$

This implies that *symplectic transformations*, that is, linear transformations $S\colon \Gamma \to \Gamma$ such that

$$S^*\Omega(\varphi_1,\varphi_2) := \Omega(S\varphi_1, S\varphi_2) = \Omega(\varphi_1,\varphi_2), \tag{2.13}$$

are $*$-automorphisms of $\mathcal{A}$ given by

$$\alpha \cdot W(\varphi) = W(S\varphi). \tag{2.14}$$

In particular, the symplectic transformation $\mathcal{T}_{(T_{\rm I},T_{\rm F})}$ representing time evolution from $T_{\rm I}(\Sigma)$ to $T_{\rm F}(\Sigma)$ defines a $*$-automorphism which we denote by $\alpha_{(T_{\rm I},T_{\rm F})}$.

Time evolution in the algebraic formulation of quantum field theory can be described as follows. Assign the state ω to the initial time as represented by the embedding $T_{\rm I}$. Thus the expectation value of the observable represented by $W \in \mathcal{A}$ on the surface $T_{\rm I}(\Sigma)$ is given by

$$\langle W \rangle_{T_{\rm I}} = \omega(W). \tag{2.15}$$

The (inverse) automorphism

$$W \longrightarrow \alpha^{-1}_{(T_{\rm I},T_{\rm F})} \cdot W \tag{2.16}$$

is the mathematical representation of time evolution of observables in the Heisenberg picture. In particular, the expectation value of $W(\varphi)$ at the final time is given by

$$\langle W(\varphi) \rangle_{T_{\rm F}} = \omega(\alpha^{-1}_{(T_{\rm I},T_{\rm F})} \cdot W(\varphi)) = \omega(W(\mathcal{T}^{-1}_{(T_{\rm I},T_{\rm F})}\varphi)) \tag{2.17}$$

Eq. (2.17) was built up using the Heisenberg picture. It is also possible to view dynamical evolution in the Schrödinger picture. This amounts to viewing the symplectic transformation $\mathcal{T}^{-1}_{(T_{\rm I},T_{\rm F})}$ as defining a change of state rather than a change in the observables. Thus if $\omega\colon \mathcal{A} \to \mathbf{C}$ is the initial state, then the final state $\omega_{T_{\rm F}}$ is defined by

$$\omega_{T_{\rm F}} = \omega \circ \alpha^{-1}_{(T_{\rm I},T_{\rm F})}. \tag{2.18}$$

It is easy to check that $\omega_{T_{\rm F}}$ is indeed a state (positive, linear, normalized). Of course, in either picture the physical output of the theory is the same. In particular, the expectation value of $W(\varphi)$ at the final time is given by (2.17) in either picture.

The foregoing description of quantum time evolution, we feel, is quite straightforward and illustrates nicely the power of the algebraic approach to quantum field theory. Our main goal here is to consider the problem of describing time evolution between arbitrary Cauchy surfaces using the more traditional apparatus of Hilbert space, linear operators, and so forth. The relation between the algebraic formulation and the Hilbert space formulation can be made via the "GNS construction", which is summarized as follows. Given any state ω_0 in the algebraic approach, there exists a Hilbert space $\mathcal{F}$ and a cyclic representation of the algebra $\mathcal{A}$ on $\mathcal{F}$ by bounded linear operators such that the cyclic vector $|\psi_0\rangle$ is related to ω_0 via

$$\omega_0(W) = \langle \psi_0 | \pi(W) | \psi_0 \rangle, \tag{2.19}$$

where $\pi(W)\colon \mathcal{F} \to \mathcal{F}$ is the operator representative of $W \in \mathcal{A}$. The Hilbert space representation associated to a given ω_0 is unique up to unitary equivalence.

If the underlying classical phase space is a symplectic vector space of finite dimension, and we use the Weyl algebra to describe the basic observables, then the GNS construction leads to a representation that is unitarily equivalent to the standard Schrödinger representation in quantum mechanics. When the phase space is infinite-dimensional, unitarily inequivalent representations can occur, depending upon the choice of ω_0. In the case of a free field propagating on Minkowski spacetime, the requirements of Poincaré invariance and positivity of energy select a unique choice of ω_0 (the vacuum state) from which the conventional Fock representation of the theory arises.

Given a Hilbert space representation of the Weyl algebra $\mathcal{A}$, one says that a symplectic transformation $S\colon \Gamma \to \Gamma$, with corresponding algebra automorphism $\alpha\colon \mathcal{A} \to \mathcal{A}$ is (unitarily) *implementable* if there is a unitary transformation $U\colon \mathcal{F} \to \mathcal{F}$ on the Hilbert space $\mathcal{F}$ such that, for any $W \in \mathcal{A}$,

$$U^{-1}\pi(W)U = \pi(\alpha \cdot W). \tag{2.20}$$

Thus, implementable transformations are those which can be represented by unitary operators on the chosen Hilbert space representation of $\mathcal{A}$.

Thanks to the uniqueness of the Hilbert space representation arising from a given ω_0 in the GNS construction, it follows that if ω_0 is invariant under S,

$$\omega_0(\alpha \cdot W) = \omega_0(W), \tag{2.21}$$

then S is implementable on the GNS Hilbert space defined by ω_0.[2] In particular, if S is the representation on Γ of a Poincaré transformation, then it is implementable in the standard Fock representation of the Klein-Gordon field theory on Minkowski spacetime.

On the other hand, in contrast to the case where the dimension of Γ is finite, not *all* symplectic transformations S will be implementable in field theory. This is because ω_0 and its transform $\omega_0 \circ \alpha$ will not always define unitarily equivalent Hilbert space representations. The central issue of this paper is the implementability of the symplectic transformation $\mathcal{T}_{(T_{\rm I},T_{\rm F})}$ (or, equivalently, $\mathcal{T}^{-1}_{(T_{\rm I},T_{\rm F})}$) on the standard Fock representation of a free field, to which we now turn.

III. FUNCTIONAL EVOLUTION OF A SCALAR FIELD ON A FLAT SPACETIME

The question of unitary implementability of symplectic transformations on Fock representations of the Weyl algebra seems to have been first answered by Shale [11]; see also [12]. The principal requirement for implementability is that the mixing between creation and annihilation operators induced by the symplectic transformation be described by a Hilbert-Schmidt operator.

Here we consider the implementability of functional evolution for a free Klein-Gordon field evolving on a flat spacetime. For technical simplicity we compactify space into a torus: $\Sigma = \mathbf{T}^n$. Standard local coordinates on M are denoted by X^α, $\alpha = 0, 1, 2, \ldots, n$, where $X^a = (X^1, X^2, \ldots, X^n) \in (0, 2\pi)$. The spacetime metric takes the form

$$g = \eta_{\alpha\beta} dX^\alpha \otimes dX^\beta, \tag{3.1}$$

where $\eta_{\alpha\beta} = \mathrm{diag}(-1, 1, 1, \ldots, 1)$.

A. Classical dynamics

Any classical solution $\varphi \in \Gamma$ to the Klein-Gordon equation on the spacetime $(\mathbf{R} \times \mathbf{T}^n, \eta)$ is of the form

[2] While (2.21) is sufficient for implementability of S, it is by no means necessary.

$$\varphi = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_k(2\pi)^n}} \left[a_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{X} - \omega_k X^0)} + a^*_{\mathbf{k}} e^{-i(\mathbf{k}\cdot\mathbf{X} - \omega_{\mathbf{k}} X^0)} \right], \tag{3.2}$$

where we use boldface to denote n-component vectors. The wave vector $\mathbf{k}$ has integer components and $\omega_k = \sqrt{k^2 + m^2}$, with $k = |\mathbf{k}|$. The Fourier coefficients $a_{\mathbf{k}}$ and $a^*_{\mathbf{k}}$ can be viewed as (complex) coordinates on the (real) phase space Γ of solutions to the Klein-Gordon equation. Since φ is smooth, the Fourier coefficients are rapidly decreasing, that is, $|a_{\mathbf{k}}|$ vanishes faster than any power of $1/k$ as $k \to \infty$.

The symplectic transformation $\mathcal{T}_{(T_{\rm I}, T_{\rm F})}$ defines, and is defined by, a transformation of $a_{\mathbf{k}}$ and $a^*_{\mathbf{k}}$. A straightforward computation establishes that

$$(\mathcal{T}_{(T_{\rm I}, T_{\rm F})} a)_{\mathbf{k}} = \sum_{\mathbf{l}} \left(\alpha_{\mathbf{kl}} a_{\mathbf{l}} + \beta_{\mathbf{kl}} a^*_{\mathbf{l}} \right), \tag{3.3}$$

where

$$\alpha_{\mathbf{kl}} = -\frac{1}{2(2\pi)^n} \frac{1}{\sqrt{\omega_k \omega_l}} \int_{\mathbf{T}^n} \left(\sqrt{\gamma_{\rm F}} n^\alpha_{\rm F} l_\alpha + \sqrt{\gamma_{\rm I}} n^\alpha_{\rm I} k_\alpha \right) e^{i(l_\alpha T^\alpha_{\rm F} - k_\alpha T^\alpha_{\rm I})} \, d^n x, \tag{3.4}$$

and

$$\beta_{\mathbf{kl}} = \frac{1}{2(2\pi)^n} \frac{1}{\sqrt{\omega_k \omega_l}} \int_{\mathbf{T}^n} \left(\sqrt{\gamma_{\rm F}} n^\alpha_{\rm F} l_\alpha - \sqrt{\gamma_{\rm I}} n^\alpha_{\rm I} k_\alpha \right) e^{-i(l_\alpha T^\alpha_{\rm F} + k_\alpha T^\alpha_{\rm I})} \, d^n x. \tag{3.5}$$

In (3.4) and (3.5) we use the following notation. The initial and final surfaces are described, respectively, by the embeddings

$$X^\alpha = T^\alpha_{\rm I}(x), \quad \text{and} \quad X^\alpha = T^\alpha_{\rm F}(x), \tag{3.6}$$

where x^i are any coordinates on $\mathbf{T}^n$. The unit normal to the initial (final) Cauchy surface is $n^\alpha_{\rm I}$ ($n^\alpha_{\rm F}$). The determinant of the metric induced on the initial (final) surface is $\gamma_{\rm I}$ ($\gamma_{\rm F}$). The normals and the induced metrics are functions of x^i (and functionals of the embedding). We set $k_\alpha = (-\omega_k, \mathbf{k})$. Our goal is to determine whether the transformation (3.3) is implementable on the usual Fock representation of the field theory, which we will now describe.

B. Quantum dynamics, the Hilbert-Schmidt condition

The principal step needed to construct an irreducible Fock representation of any linear field theory defined by a symplectic vector space (Γ, Ω) is the selection of a suitable scalar product $\mu\colon \Gamma \times \Gamma \to \mathbf{R}$ on Γ satisfying [13,14]

$$\mu(\varphi_1, \varphi_1) = \frac{1}{4} \sup_{\varphi_2 \neq 0} \frac{[\Omega(\varphi_1, \varphi_2)]^2}{[\mu(\varphi_2, \varphi_2)]}, \quad \forall\, \varphi_1 \in \Gamma. \tag{3.7}$$

Given such an inner product μ, there exists a (complex) Hilbert space $\mathcal{H}$, equipped with a scalar product (,), and a real-linear mapping $K\colon \Gamma \to \mathcal{H}$ with dense range, such that

$$(K\varphi_1, K\varphi_2) = \mu(\varphi_1, \varphi_2) - \frac{i}{2}\Omega(\varphi_1, \varphi_2). \tag{3.8}$$

The space $\mathcal{H}$ is the "one-particle Hilbert space". The Fock space arises from $\mathcal{H}$ via tensor products and direct sums as usual. On the Fock space the Weyl algebra is represented via (densely defined, self-adjoint) field operators built from creation and annihilation operators in the standard way. From the point of view of the algebraic approach, the choice of inner product μ defines the Fock representation via the GNS construction based upon a state ω_0, which is defined on the basic generators by

$$\omega_0(W(\varphi)) = e^{-\frac{1}{2}\mu(\varphi,\varphi)}, \tag{3.9}$$

and is extended to the whole algebra by linearity and continuity. In this context, (3.7) implies that ω_0 is a positive function on the Weyl algebra.

In terms of the expansion (3.2), the scalar product μ we use to quantize the Klein-Gordon field on $\mathbf{R} \times \mathbf{T}^n$ is given by

$$\mu(\varphi_1, \varphi_2) = \frac{1}{2}\sum_{\mathbf{k}} \left(a^*_{1\mathbf{k}} a_{2\mathbf{k}} + a_{1\mathbf{k}} a^*_{2\mathbf{k}}\right). \tag{3.10}$$

This is simply the discrete momentum version of the usual choice made in the standard Poincaré invariant quantization of the Klein-Gordon field on Minkowski spacetime. In Appendix A we indicate that the time evolution mapping $\mathcal{T}$ is bounded (continuous) in this norm. This result is necessary for unitary implementability of the transformation [14]. It also means that complications due to operator domain considerations do not arise.

Using the norm (3.10), the one particle Hilbert space $\mathcal{H}$ can be identified with the complex functions

$$\psi = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_k (2\pi)^n}} a_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{X} - \omega_k X^0)} \tag{3.11}$$

for which

$$\sum_{\mathbf{k}} |a_{\mathbf{k}}|^2 < \infty. \tag{3.12}$$

Thus $\mathcal{H}$ is the set of "positive frequency" solutions to the Klein-Gordon equation with finite "Klein-Gordon norm". The mapping $K\colon \Gamma \to \mathcal{H}$ mentioned above is given by

$$K\varphi = \psi, \tag{3.13}$$

with φ defined by (3.2) and ψ defined by (3.11).

The bounded transformation (3.3) defines a pair of bounded linear maps, $\alpha : \mathcal{H} \to \mathcal{H}$ and $\beta : \mathcal{H} \to \bar{\mathcal{H}}$, where $\bar{\mathcal{H}}$ is the complex conjugate space to $\mathcal{H}$. With ψ given by (3.11), we have

$$\alpha \cdot \psi = \sum_{\mathbf{k},\mathbf{l}} \frac{1}{\sqrt{2\omega_k (2\pi)^n}} \alpha_{\mathbf{kl}}\, a_{\mathbf{l}}\, e^{i(\mathbf{k}\cdot\mathbf{X} - \omega_k X^0)}. \tag{3.14}$$

and

$$\beta \cdot \psi = \sum_{\mathbf{k},\mathbf{l}} \frac{1}{\sqrt{2\omega_k (2\pi)^n}} \beta^*_{\mathbf{kl}}\, a_{\mathbf{l}}\, e^{-i(\mathbf{k}\cdot\mathbf{X}-\omega_k X^0)}. \tag{3.15}$$

These transformations constitute the familiar Bogolubov transformation associated to any symplectic transformation on the classical phase space. The results of Refs. [11,12] on unitary implementability state that a bounded symplectic transformation, such as the time evolution map $\mathcal{T}$, is implementable on the Fock space if and only if the operator $\beta\colon \mathcal{H} \to \bar{\mathcal{H}}$ is Hilbert-Schmidt, that is,

$$\mathrm{tr}(\beta^\dagger \beta) = \sum_{\mathbf{k},\mathbf{l}} |\beta_{\mathbf{lk}}|^2 < \infty. \tag{3.16}$$

We now show that this condition is, in general, *not* satisfied if the spacetime dimension is greater than 2. We first give an outline of the computations, then we present details of an illustrative special case. We give further details in Appendix B.

For simplicity, we will restrict attention to the case where the initial surface is fixed and the final surface is kept arbitrary (that is, kept variable). We fix the initial surface to be $X^0 = 0$ with standard spatial coordinates. Thus

$$T^\alpha_{\mathrm{I}}(x) = (0, x^a). \tag{3.17}$$

We consider the validity of the Hilbert-Schmidt condition (3.16) for an arbitrary final Cauchy surface. The sum in (3.16) is convergent if and only if it is absolutely convergent. Hence, to show violation of the Hilbert-Schmidt condition, it suffices to show that a sub-sum diverges. Our strategy is to consider the large k behavior of a sub-sum over $\mathbf{k}$ in which $\frac{l}{k} = O(1)$ is held fixed. In such a sub-sum, the Bogolubov coefficients $\beta_{\mathbf{lk}}$ to leading order in k turn out to be of the form

$$\beta_{\mathbf{lk}} = \int_{\mathbf{T}^n} e^{-ikG(\mathbf{x},\Omega_{\mathbf{k}})} h(\mathbf{x},\Omega_{\mathbf{k}})\, d^n x, \tag{3.18}$$

where $\Omega_{\mathbf{k}}$ are the angular components of $\mathbf{k}$. The functions G and h depend upon the choice of embedding.

Eq. (3.18) can be estimated by the method of stationary phase [15]. The estimate, for a large class of embeddings (namely those for which the condition $\frac{\partial G}{\partial x^i} = 0$ is satisfied at a finite number of points $\mathbf{x}_I$,[3] $I = 1, 2, \ldots, N$, and the second derivative matrix $\frac{\partial^2 G}{\partial x^i \partial x^j}$ has non zero determinant D at $\mathbf{x}_I$), is

$$\beta_{\mathbf{lk}} = \left(\frac{2\pi}{k}\right)^{\frac{n}{2}} \sum_{I=1}^{N} f_I e^{-ikG_I}, \tag{3.19}$$

where

[3]Note that in general, the $\mathbf{x}_I$, depend on $\Omega_{\mathbf{k}}$.

$$f_I := |D_I|^{-\frac{1}{2}} h(\mathbf{x}_I, \Omega_{\mathbf{k}}) e^{i\pi \operatorname{sign} D_I/4}, \tag{3.20}$$

$$G_I := G(\mathbf{x}_I, \Omega_{\mathbf{k}}), \quad D_I = D(\mathbf{x}_I, \Omega_{\mathbf{k}}). \tag{3.21}$$

For $n = 1$, it turns out that $h(\mathbf{x}_I, \Omega_{\mathbf{k}}) = 0$ and our subsequent arguments for non-unitarity are not valid. But for generic embeddings with $n > 1$, we have $h(\mathbf{x}_I, \Omega_{\mathbf{k}}) \neq 0$, and then

$$\sum_{\mathbf{k},\mathbf{l}} |\beta_{\mathbf{lk}}|^2 > \sum_{\mathbf{k},\, k\to\infty} \frac{1}{k^n} |\sum_{I=1}^{N} f_I e^{-ikG_I}|^2 \quad \sim \int^{\infty} \frac{d^n k}{k^n} |\sum_{I=1}^{N} f_I e^{-ikG_I}|^2. \tag{3.22}$$

Note that it is possible for $G_I = G_J$ for some $I \neq J$. By suitably redefining the f_I, with the redefined f_I denoted by $\tilde{f}_I$, the sum $\sum_{I=1}^{N} f_I e^{-ikG_I}$ can be rewritten as a sum over a finite number $\tilde{N} \leq N$ of terms, each of the form

$$\tilde{f}_I e^{-ik\tilde{G}_I}, \quad I = 1, 2, \ldots, \tilde{N}, \quad \tilde{G}_I \neq \tilde{G}_J \text{ for } I \neq J. \tag{3.23}$$

For generic embeddings, at least one of the $\tilde{f}_I$ is non-zero. We restrict attention to such embeddings. Then

$$\sum_{\mathbf{k},\mathbf{l}} |\beta_{\mathbf{lk}}|^2 > \int_{k\to\infty} \frac{d^n k}{k^n} |\sum_{I=1}^{\tilde{N}} \tilde{f}_I e^{-ik\tilde{G}_I}|^2$$

$$= \int d\Omega_{\mathbf{k}} \int^{\infty} \frac{dk}{k} (\sum_I |\tilde{f}_I|^2 + \sum_{I\neq J} \tilde{f}_I \tilde{f}_J^* e^{-ik(\tilde{G}_I - \tilde{G}_J)}). \tag{3.24}$$

The integral over k of the second ($I \neq J$) summation converges, as can be seen using integration by parts and (3.23). The remaining integral, $\int \frac{dk}{k}(\sum_I |\tilde{f}_I|^2)$, diverges logarithmically with k and hence β is not Hilbert-Schmidt, that is, the evolution is not implementable.

In what immediately follows, we use the above type of computation to demonstrate that β is not Hilbert-Schmidt for an illustrative special case in which the final slice is non-trivial ($X^0 \neq$ *const.* on this slice) but the coordinates on it are the restrictions of the spatial Minkowskian coordinates, $T_{\rm F}^a(x) = x^a$. We shall refer to this as the "no spatial diffeomorphism" case. The most general final slice would also allow for an arbitrary set of spatial coordinates. In Appendix B we extend the proof to that more general case. The discussion there has two parts. First we consider a case that is, in a sense, the exact opposite of the "no spatial diffeomorphism" case: the final slice is chosen to be $X^0 = 0$, so that no real time evolution has taken place, but the coordinates on the final slice are arbitrary. In other words, the final slice differs from the initial slice by a spatial diffeomorphism only. We shall refer to this as the "pure spatial diffeomorphism" case. We find that the pure spatial diffeomorphism case also has the property that β is not Hilbert-Schmidt. Finally, we indicate how to combine the non-implementability results from the "no spatial diffeomorphism" and "pure spatial diffeomorphism" cases to the general case of nontrivial final slice and arbitrary spatial coordinates.

In the no spatial diffeomorphism case, the initial surface has embedding $T_{\rm I}^\alpha(x) = (0, x^a)$ and the final surface has embedding

$$T_{\rm F}^\alpha = (f(\mathbf{x}), x^a). \tag{3.25}$$

The function $f\colon \mathbf{T}^n \to \mathbf{R}$ is smooth and satisfies

$$\delta^{ij}(\partial_i f)(\partial_j f) \equiv (\vec{\nabla} f)\cdot(\vec{\nabla} f) < 1, \tag{3.26}$$

so that the final surface is everywhere spacelike. On the final surface we have

$$\sqrt{\gamma_{\rm F}}\, n^\alpha_{\rm F} k_\alpha = -\omega_k + \mathbf{k}\cdot\vec{\nabla} f. \tag{3.27}$$

Using this relation, in conjunction with an integration by parts in (3.5), we find (after dropping an irrelevant numerical factor)

$$\beta_{\mathbf{lk}} = \frac{1}{\sqrt{\omega_k \omega_l}}\,\frac{\omega_k\omega_l + \mathbf{l}\cdot\mathbf{k} - m^2}{\omega_k}\int_{\mathbf{T}^n} e^{-i(\mathbf{l}+\mathbf{k})\cdot\mathbf{x} + i\omega_k f}\, d^n x. \tag{3.28}$$

We now consider the behavior of $\beta_{\mathbf{lk}}$ for large k with $\frac{l}{k}$ fixed and of order unity. We have

$$\beta_{\mathbf{lk}} = \beta^{(1)}_{\mathbf{lk}} + \beta^{(2)}_{\mathbf{lk}}, \tag{3.29}$$

where

$$\beta^{(1)}_{\mathbf{lk}} := \int_{\mathbf{T}^n} h\, e^{-ikG}\, d^n x\ , \tag{3.30}$$

$$\beta^{(2)}_{\mathbf{lk}} := \int_{\mathbf{T}^n} O(\frac{1}{k}) e^{-ikG}\, d^n x, \tag{3.31}$$

with

$$G := \frac{\mathbf{l}+\mathbf{k}}{k}\cdot\mathbf{x} - f\ , \tag{3.32}$$

$$h := \sqrt{\frac{l}{k}}(1 + \frac{\mathbf{l}\cdot\mathbf{k}}{lk})\ . \tag{3.33}$$

We estimate the large k behavior of (3.30) by the stationary phase method [15]. The stationary points of $G(\mathbf{x})$ are points such that, for given values of $\mathbf{l}/k$ and $\Omega_{\mathbf{k}}$,

$$\frac{\partial G}{\partial x^i} = 0 \quad \Rightarrow \quad \frac{\partial f}{\partial x^i} = \frac{l_i}{k} + \frac{k_i}{k}. \tag{3.34}$$

In order to allow critical points of G to exist, we confine our attention to points in **k**-**l** space such that $|\mathbf{l}+\mathbf{k}|^2 < k^2$. We focus on the sub-sum of (3.16) obtained by fixing $\frac{\mathbf{l}}{k} =: \mathbf{L}$ and allowing $\frac{\mathbf{k}}{k}$ to vary in an open neighborhood of a fixed unit vector $\mathbf{K}$. To ensure that our approximation (3.24) works, we demand that the embedding (and the choice of $\mathbf{L}$ and $\mathbf{K}$) be such that the following 'genericity' conditions hold.

(i) There exist only a finite number of points $\mathbf{x}_I$, $I = 1, \ldots, N$ on the slice where $\vec{\nabla} f = \mathbf{L}+\mathbf{K}$.

(ii) the matrix $\frac{\partial^2 f}{\partial x^i \partial x^j}$ evaluated at $\mathbf{x}_I$ have non-zero determinant.

(iii) h given by (3.33), when evaluated at $\mathbf{l} = k\mathbf{L}$ and $\mathbf{k} = k\mathbf{K}$, is non zero.

(iv) At least one $\tilde{f}_I$ in (3.23) be non zero.

Conditions **(i)** and **(ii)** imply that there exist a fixed, finite number of critical points of G for each term in the sub-sum. In particular, we note that at fixed $\mathbf{L}$, (3.34) defines a map $\lambda\colon \mathbf{T}^n \to \mathbf{R}^n$ taking $\mathbf{x} \in \mathbf{T}^n$ to $\frac{\mathbf{k}}{k} \in \mathbf{R}^n$. From this point of view, **(ii)** states that the differential of λ is non-degenerate at the critical points of G. An application of the inverse mapping theorem to λ implies that (a) the number of critical points N does not change as $\frac{\mathbf{k}}{k}$ varies in a sufficiently small neighborhood of $\mathbf{K}$, and (b) the location of the critical points varies continuously with $\frac{\mathbf{k}}{k}$ (in a neighborhood of $\mathbf{K}$). The results (a) and (b) ensure that the explicit expression (3.24) holds. Conditions **(iii)** and **(iv)** ensure that the contribution of the critical points is non-trivial.

Any embedding which satisfies the requirements **(i)**-**(iv)**, has an associated β_1 which is not Hilbert-Schmidt as can be seen by the arguments following (3.18). The same arguments show that β_2 contributes only convergent terms to the relevant sub-sum over $|\beta_{\mathbf{lk}}|^2$. Hence, β is not Hilbert-Schmidt.

We remark that there are two special cases where our proof of the failure of (3.16) does not apply because not all of the conditions **(i)**–**(iv)** are satisfied. First, if f is a constant (so that the final slice is just a time translation of the initial slice, which is clearly implementable) then all of the conditions fail to be satisfied. Second, the condition (3.26) that the embedding be spacelike, in conjunction with **(i)**, implies that $|\mathbf{K}+\mathbf{L}| < 1$, and it follows that $\mathbf{K}\cdot\mathbf{L} < 0$. When $n = 1$, this means that **(iii)** is not satisfied. Indeed, it is shown in [6] that functional evolution is unitarily implemented when $n = 1$.

When $n > 1$, the conditions **(i)**, **(ii)**, **(iv)** are rather weak restrictions on the final embedding. Moreover, these conditions are probably stronger than necessary. For example, if **(ii)** fails, we may expect the large k behavior of $\beta_{\mathbf{lk}}$ to be even more divergent [15].

IV. DISCUSSION

We have shown that dynamical evolution of a free field on a flat spacetime with topology $\mathbf{R} \times \mathbf{T}^n$ will not be unitarily implemented if the initial hypersurface is flat and the final hypersurface is suitably generic. There is no reason to expect that the situation will be improved by allowing for a more general (but generic) initial surface. It is not the curvature *per se* of the final (and/or initial) surface which causes the problem with unitarity, but rather that, in general, there is no isometry of the spacetime that will map the initial surface to the final surface. Indeed, it is easy to see that evolution between any two Cauchy surfaces related by an isometry *is* unitarily implemented. This situation is analogous to the Van Hove obstruction to unitary implementability of the group of canonical transformations [16], which indicates that only a subset of the group of canonical transformations can be represented as unitary transformations in quantum mechanics. In our case, the canonical transformations defined by the isometry group of the spacetime are unitarily represented, but canonical transformations induced by more general mappings of the spacetime onto itself are not unitarily implemented.

While we have chosen to work with a compactified model of space, we do not expect our result (failure of unitarity of functional evolution) to change if we the take the limit as the torus fills out $\mathbf{R}^n$. Indeed, the failure of the Hilbert-Schmidt condition for $n > 1$ is an ultraviolet effect (by computing on $\mathbf{R} \times \mathbf{T}^n$, we have tacitly ruled out infrared effects), and should be insensitive to the topology of the spatial manifold. Thus we expect that functional evolution will not be unitarily implemented on Minkowski spacetime. Of course, dynamical evolution between any two surfaces related by a Poincaré transformation will be unitarily implemented on the standard free field Fock space, but this appears to be as far as one can go. One could attempt to improve this situation by considering more exotic representations of the CCR. If functional evolution could be unitarily implemented in this way, it would certainly be interesting, at least mathematically. But physically one is forced to adopt the Poincaré invariant quantization scheme and the concomitant failure of unitarity of functional evolution.

The most pronounced implication of our results is that the Schrödinger picture is not available to describe functional evolution of free fields in flat spacetime using the traditional Fock space formulation of the quantum theory. The difficulties that arise in the functional evolution formalism are, apparently, more fundamental than envisioned by Dirac, who worried about integrability of evolution between arbitrary Cauchy surfaces. More precisely, Dirac was concerned with the difficulty in defining the Tomonaga-Schwinger equation in such a way that evolution from an initial surface to a final surface is independent of the choice of foliation used to interpolate between the initial and final surfaces. Given that the evolution between initial and final surfaces is not defined by a unitary transformation, it seems impossible to make rigorous sense of the Tomonaga-Schwinger equation[4] (in the Schrödinger picture) and so issues of integrability of this equation appear to be academic. We note that if the Schrödinger picture of functional evolution is problematic, the Heisenberg picture is still available. It should be kept in mind, though, that in the Heisenberg picture one does not have a unitary operator to evolve the fields between arbitrary Cauchy surfaces.

Unfortunately, in applications of the functional evolution formalism to canonical quantum gravity one *is* working in the Schrödinger picture. In particular, the weak field and/or semi-classical limits of the Wheeler-DeWitt equation (or its Ashtekar variables counterpart) can be shown — formally — to yield a Tomonaga-Schwinger equation describing the propagation of the Schrödinger picture state function for fields on a fixed background spacetime [17]. This feature of the Wheeler-DeWitt equation has been viewed as a valuable (if formal) "sanity check" on the Dirac approach to canonical quantization of the gravitational field. The problematic nature of the functional evolution formulation of dynamics in a Hilbert space setting indicates that the weak field/semi-classical limits of the Wheeler-DeWitt equation cannot, strictly speaking, be well-defined in terms of a Hilbert space of states. Perhaps one can even infer that the Wheeler-DeWitt equation itself cannot be well-defined as an equation selecting a Hilbert space of physical states. After all, if one cannot sensibly describe functional evolution of a free field in flat spacetime using a Hilbert space of states, it be-

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[4]We say this since the existence of a self-adjoint generator of time evolution, such as is needed to define the Schrödinger equation, is equivalent to having a continuous 1-parameter unitary group. Strictly speaking, this result does not apply to functional evolution since such evolution cannot be described as a 1-parameter group. But one does not expect the situation to improve when the group assumption is dropped.

comes questionable whether it can be done in non-perturbative canonical quantum gravity. Nevertheless, our feeling is that such a point of view is overly pessimistic. Current proposals for defining a Hilbert space of states for quantum gravity seem very different from Fock representations of free field theory [18]. Moreover, while the semi-classical and/or weak field limits may formally appear in terms of functional evolution of free fields, there may be built-in limitations to these approximations from the underlying non-perturbative description. Indeed, the difficulties we have uncovered with functional evolution are ultraviolet problems; strong field/non-perturbative effects should be playing a role in the ultraviolet regime.

In any case, we have seen that the algebraic approach to quantum field theory does not appear to have any difficulties accommodating functional evolution, at least for free fields on a fixed background spacetime. Indeed, problems analogous to those we encountered with functional evolution played a role in motivating the development of the algebraic formalism. Thus the results presented here provide some support for an algebraic approach to quantization of constrained Hamiltonian field theories such as arise in general relativity. In such an approach the appropriate weak field and/or semi-classical limit would yield a functional evolution formalism such as is outlined in section **II**.

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APPENDIX A: TIME EVOLUTION IS CONTINUOUS

Here we show that the time evolution map $\mathcal{T}$ on the phase space of a Klein-Gordon field on the flat spacetime $\mathbf{R}\times\mathbf{T}^n$ is bounded (*i.e.*, continuous) in the norm $||\varphi||^2 = \mu(\varphi,\varphi)$. This is equivalent to saying that the Bogolubov transformation operators α and β on the one-particle Hilbert space are bounded (continuous) maps. This result is necessary for unitary implementability [14]. That $\mathcal{T}$ is bounded is also very convenient since it means that complicated operator domain issues do not arise.

We will establish that there is a constant C such that, for all $\varphi\in\Gamma$,

$$||\mathcal{T}\varphi|| \leq C||\varphi|| \tag{A1}$$

To begin, it is useful to have the norm $||\cdot||$ expressed in terms of Cauchy data, that is, as a norm on the space Υ. For simplicity, we identify Υ and Γ using a flat surface with standard spatial coordinates; the embedding is $T^\alpha(x) = (0, x^a)$. In terms of Cauchy data (ϕ,π) on this surface we have

$$||\varphi||^2 =<\pi, \Lambda^{-1}\pi> + <\phi, \Lambda\phi>, \tag{A2}$$

where $<\cdot,\cdot>$ is the L^2 inner-product on $\mathbf{T}^n$, and

$$\Lambda = \sqrt{\Delta + m^2}. \tag{A3}$$

Here $\Delta = -\delta^{ij}\partial_i\partial_j$ is the Laplacian defined by the induced metric on the $X^0 = 0$ surface. A convenient form of this norm is as follows. Define

$$u_1 = \Lambda\phi, \quad u_2 = \pi. \tag{A4}$$

We now have

$$||\varphi||^2 = < u_1, \Lambda^{-1}u_1 > + < u_2, \Lambda^{-1}u_2 > . \tag{A5}$$

We write $u = (u_1, u_2)$. It is easy to see that $||\cdot||$ is equivalent to a Sobolev norm $||\cdot||_{-1/2}$ [19] on the space of fields $u = (u_1, u_2)$.

We now proceed as follows. We first consider the time evolution map $\mathcal{T}$ from a flat initial surface to an arbitrary (but non-intersecting) final surface. We will indicate below that this particular time evolution map is bounded in the norm (A5). It is easy to see that this result implies the corresponding Bogolubov operators α and β are bounded as well. This implies that the Bogolubov operators for the inverse transformation (which are defined in terms of α, β and their adjoints) are bounded, which implies that $\mathcal{T}^{-1}$ is bounded. Now, the general time evolution map from $T_1(\Sigma)$ to $T_2(\Sigma)$, with these Cauchy surfaces arbitrary, can be obtained by evolving from $T_1(\Sigma)$ to a flat slice (using $\mathcal{T}^{-1}$) and then evolving from the flat slice to $T_2(\Sigma)$ (using $\mathcal{T}$). Since both of these evolution maps are bounded so is their composition and hence the general time evolution map between any two surfaces is bounded.

The argument in the preceding paragraph reduces our task to showing that time evolution is a bounded map when considering evolution from an initial Cauchy surface with embedding $T^\alpha(x) = (0, x^a)$ to any final Cauchy surface with arbitrary embedding. Let us introduce a foliation by Cauchy surfaces, which are labeled by t, that interpolates between the initial flat embedding at $t = 0$ and the final embedding at $t = t'$. We have to compare the norms of solutions φ and $\mathcal{T}\varphi$ where the Cauchy data at $t = 0$ for $\mathcal{T}\varphi$ are the Cauchy data for φ at $t = t'$. By translating the Klein-Gordon equation into coordinates adapted to the given foliation, it is easy to see that to any $\varphi \in \Gamma$ there corresponds a 1-parameter set of functions $u(t) = (u_1(t), u_2(t))$, related to the Cauchy data at time t via (A4), and satisfying a set of strictly hyperbolic evolution equations on the chosen foliation (see [19] for the definition of strictly hyperbolic). The solutions of the Klein-Gordon equation, φ and $\mathcal{T}\varphi$, respectively correspond to solutions u and $\mathcal{T}u$ of the evolution equations, where $(\mathcal{T}u)(0) = u(t')$.

From this line of reasoning we see that we want to compare the Sobolev norms $||u(0)||$ and $||(\mathcal{T}u)(0)|| = ||u(t')||$. Because the evolution equations are strictly hyperbolic we have the following estimate (valid for any Sobolev norm) [19],

$$||u(t')|| \leq C||u(0)||.$$

From our discussion above, this implies (A1). Thus, time evolution from any initial Cauchy surface to any final Cauchy surface is a bounded, that is, continuous mapping in the norm defined by μ in (3.10). This also means that the norms $||\varphi||$ and $||\varphi||_{\mathcal{T}} \equiv ||\mathcal{T}\varphi||$ are equivalent.

APPENDIX B: THE PURE SPATIAL DIFFEOMORPHISM CASE AND THE GENERAL CASE

Here we complete the proof of failure of functional evolution to be implementable by extending our analysis from III to the pure spatial diffeomorphism case and the general case.

1. The pure spatial diffeomorphism case

Here the time evolution is trivial in the sense that the initial and final Cauchy surfaces are identical. The map $\mathcal{T}$ is obtained by considering initial and final embeddings that differ only by the choice of coordinates on the slice. In invariant language, the two embedded hypersurfaces differ by a spatial diffeomorphism only. In this section we show that the spatial diffeomorphisms are not unitarily represented on the Fock space of a free Klein-Gordon field.

The initial embedding is taken to be flat with standard coordinates:

$$T^{\alpha}_{\text{I}}(x) = (0, x^a). \tag{B1}$$

The final embedding is the same surface, but in coordinates $y^a = y^a(x)$:

$$T_{\text{F}}(x) = (0, y^a(x)). \tag{B2}$$

The formula (3.5) for $\beta_{\mathbf{lk}}$ takes the form (we drop an irrelevant constant factor)

$$\beta_{\mathbf{lk}} = \frac{1}{\sqrt{\omega_k \omega_l}} \int_{\mathbf{T}^n} \left(-\sqrt{\gamma}\omega(\mathbf{k}) + \omega(\mathbf{l})\right) e^{-i(\mathbf{l}\cdot\mathbf{x}+\mathbf{k}\cdot\mathbf{y})}\, d^n x. \tag{B3}$$

A coordinate change from x to y in the integral yields

$$\beta_{\mathbf{lk}} = \pm\frac{1}{\sqrt{\omega_k \omega_l}} \int_{\mathbf{T}^n} \left(-\omega(\mathbf{k}) + |\det\chi|\omega(\mathbf{l})\right) e^{-i(\mathbf{l}\cdot\mathbf{x}+\mathbf{k}\cdot\mathbf{y})}\, d^n y. \tag{B4}$$

Here we view $x^i = x^i(y)$, and we have defined

$$\chi^i_j := \frac{\partial x^i}{\partial y^j}. \tag{B5}$$

The sign of β (which is irrelevant for the Hilbert-Schmidt condition) depends upon whether the spatial diffeomorphism is orientation preserving.

As in III, for large k and $\frac{l}{k} = O(1)$ equations (3.29), (3.30) and (3.31) hold, but G and h are now given by

$$G := \frac{\mathbf{l}}{k}\cdot\mathbf{x} + \frac{\mathbf{k}}{k}\cdot\mathbf{y}\ , \tag{B6}$$

$$h := \sqrt{\frac{k}{l}}\left(-1 + |\det\chi|\,\frac{l}{k}\right)\ . \tag{B7}$$

At critical points of G,

$$\left.\frac{\partial G}{\partial y^i}\right| = 0 \quad \Rightarrow \quad \chi_i^j\, l_j = -k_i. \tag{B8}$$

As in III, we fix $\frac{\mathbf{l}}{k} = \mathbf{L}$ and vary $\frac{\mathbf{k}}{k}$ in a neighborhood of a fixed unit vector $\mathbf{K}$. We demand that the spatial diffeomorphism (and the choice of $\mathbf{L}, \mathbf{K}$) be such that the following properties hold.
(i) $\chi_i^j L_j = -K_i$ only at a finite number of points $\mathbf{y}_I, I = 1, \ldots, N$ on the slice.
(ii) The matrix $\frac{\partial^2 G}{\partial y^i \partial y^j} = \frac{\partial^2 x^m}{\partial y^i \partial y^j} L_m$ evaluated at $\mathbf{y}_I$ have non-zero determinant.
(iii) At these points, h (given by (B7)) evaluated at $\mathbf{l} = k\mathbf{L}$, $\mathbf{k} = k\mathbf{K}$ is nonzero.
(iv) There exists at least one $\tilde{f}_I$ in (3.23) that is non zero.

Any embedding which satisfies these requirements has an associated β_1 which is not Hilbert-Schmidt as can be seen by the arguments following (3.18). The role of **(i)**-**(iv)** is exactly the same as in the no spatial diffeomorphism case. Moreover, the same arguments as in the no spatial diffeomorphism case also show that β_2 contributes only convergent terms to the relevant sub sum over $|\beta_{\mathbf{lk}}|^2$. Hence, β is not Hilbert-Schmidt.

We remark that if χ_i^j is a constant matrix, then not all the conditions **(i)**–**(iv)** are satisfied. In particular, if the spatial diffeomorphism is simply a translation (which is clearly implementable), then all of the conditions fail to be satisfied. Note also that, for $n = 1$, condition **(iii)** is always violated. To see this, use (B8) to get (when $n = 1$)

$$|\det \chi|(\mathbf{y}_I) = \frac{k}{l}, \tag{B9}$$

which implies that $h(y_I) = 0$.

2. The general case

Here we combine the arguments and use the notation of the "no spatial diffeomorphism" and "pure spatial diffeomorphism" cases. As usual, we use

$$T^\alpha_{\mathrm{I}}(x) = (0, x^i) \quad \text{and} \quad T^\alpha_{\mathrm{F}}(x) = (f(\mathbf{x}), y^i(\mathbf{x})) \tag{B10}$$

in (3.5). Make the coordinate change from x to y. Then, using the fact that $\sqrt{\gamma} n^\alpha k_\alpha$ is of density weight 1 and the results of the previous two special cases, we get

$$\beta_{\mathbf{lk}} = \frac{1}{\sqrt{\omega_k \omega_l}} \int_{\mathbf{T}^n} \left(-\omega_k + \mathbf{k}\cdot\vec{\nabla} f + \chi\omega_l\right) e^{-i(\mathbf{l}\cdot\mathbf{x}+\mathbf{k}\cdot\mathbf{y})+i\omega_k f(\mathbf{y})}\, d^n x. \tag{B11}$$

Equations (3.29), (3.30) and (3.31) hold with

$$G := \frac{1}{k}(\mathbf{l}\cdot\mathbf{x} + \mathbf{k}\cdot\mathbf{y}) - f(y) \tag{B12}$$

$$h := \sqrt{\frac{k}{l}}(-1 + \frac{\mathbf{k}}{k}\cdot\vec{\nabla} f + \chi\frac{l}{k})\,. \tag{B13}$$

The critical points of G are obtained via,

$$\chi^i_j \frac{l_i}{k} + \frac{k_j}{k} - \frac{\partial f}{\partial y^j} = 0. \tag{B14}$$

We use $\mathbf{L}$ and $\mathbf{K}$ as in the pure diffeomorphism and no diffeomorphism cases. We demand that the embedding and the choice of $\mathbf{L}$ and $\mathbf{K}$ be such that the following properties hold.
(i) There are only a finite number of points y_I, $I = 1, 2, \ldots, N$ where $\chi^i_j L_i - \frac{\partial f}{\partial y^j} = -K_j$.
(ii) At the points y_I, the matrix $\frac{\partial^2 G}{\partial y^i \partial y^j} = L_m \frac{\partial^2 x^m}{\partial y^i y^j} - \frac{\partial^2 f}{\partial y^i y^j}$ has non zero determinant.
(iii) At y_I, h, as given by (B13), when evaluated at $\mathbf{l} = k\mathbf{L}$ and $\mathbf{k} = k\mathbf{K}$ is non zero.
(iv) At least one of the $\tilde{f}_I$ in (3.23) be non zero.

Any embedding which satisfies these requirements has an associated β which is not Hilbert-Schmidt. The role of **(i)**–**(iv)** is the same as in the no diffeomorphism and pure diffeomorphism cases. Note that not all the conditions are satisfied when $n = 1$ or if T_{F} is a spacetime translation of T_{I}.

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