The Hamiltonians of Linear Quantum Fields: 
I. Existence Theory for Scalar Fields

Adam D. Helfer
Department of Mathematics
University of Missouri
Columbia, MO 65211, U.S.A.

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Abstract

For linear scalar field theories, I characterize those classical Hamiltonian vector fields which have self-adjoint operators as their quantum counterparts. As an application, it is shown that for a scalar field in curved space–time (in a Hadamard representation), a self-adjoint Hamiltonian for evolution along the unit timelike normal to a Cauchy surface exists only if the second fundamental form of the surface vanishes identically.

1 Introduction

When does a symmetry of a classical field theory pass over to the corresponding quantum theory?

Even for linear theories, the answer to this question is not known in the generality one would like. For finite motions, indeed, the answer is well-known: a canonical transformation of the classical phase space induces a Bogoliubov transformation on the field operators, and this transformation is unitarily implementable if and only if the Bogoliubov coefficients satisfy a certain square-summability condition (Shale 1962). However, the most important canonical transformations are those corresponding to evolution in time. For these, one almost never has an explicit knowledge of the finite transformations — getting these would involve solving the equations of motion. What one has is knowledge of the generator of the transformations — the equation of motion, or equivalently the classical Hamiltonian function or vector field. One would like to be able to read off from this whether or not the quantum evolution will be unitarily implementable. It is this problem which is solved, for scalar fields, in this paper. The analysis of other boson fields is parallel. Subsequent papers in this series will explore the structure of the Hamiltonians more fully, and treat fermions.

In the past few years, it has become apparent that this issue is important, because evidence has accumulated which strongly suggests that in generic circumstances the Hamiltonians are not self-adjointly implementable. Indeed, this appears to be one of a family of related phenomena, which at least superficially are severely pathological. They are all local, and can be expressed as certain ultraviolet divergences.
The most extreme of these phenomena is that, generically, the expectations of the energy and of the energy density are unbounded below. Schematically,

\[
\text{lower bound of } \hat{H} = (\text{finite term}) + (\text{geometric term})(-\infty),
\]

where the “geometric term” vanishes in Minkowski space but is generically non-zero. What this means is that, at least as far as the mathematical structure of the theory is concerned, the case of evolution along a covariantly constant timelike vector field in Minkowski space is a highly unstable point.

It would be hard to overstate the potential significance of this issue. It raises fundamental questions of stability and interpretation. For example, why do not perturbations send the quantum field cascading through more and more negatively energetic states, with a corresponding release of positive-energy radiation? The expectation of the energy density is used as a source term in “semiclassical gravity,” which is perhaps the most important application of quantum field theory in curved space–time. (It is this theory, for example, which predicts the loss of energy from black holes via the Hawking mechanism.) How credible is this semiclassical approximation, in view of the unboundedness-below?

These matters are at present imperfectly understood. There is a plausible resolution for them in the case of special-relativistic quantum fields, but in the case of quantum fields in curved space–time, if a similar picture is to hold, we seem to have to confront quantum fluctuations in the geometry in an essential way. I shall outline this picture below. It must be emphasized, though, that at present, even in the special-relativistic case, the picture is one of physical plausibility. To justify (or negate) it, one needs a firm understanding of what the mathematical structure is. The main aim of the present series of papers is to lay the foundations of the general theory of the Hamiltonians involved.

The Emerging Picture Workers in the theory of quantum fields in time-dependent external potentials have been aware of some of the issues raised here for some time, but the ideas have been surprising to workers in quantum field theory in curved space–time. I should like to explain here what the significance of these issues is, and in particular why, for quantum fields in curved space–time, they may be of the deepest significance. I will also try to give a modern point of view of the state of affairs for special-relativistic quantum fields in time-dependent external potentials.

Of course, any attempt to say what picture is “emerging” before it has actually emerged involves some judgments, which may not be shared with all workers. I shall comment in particular on the relation between the view here the “algebraic approach,” below.

Failure of Unitary Implementability I shall first discuss the non-unitarities, that is, the failure of evolution of the field for finite times to be unitarily implementable.\(^1\) While the present papers are really concerned with the Hamiltonians (that is, evolution for infinitesimal time), one should understand the significance of the non-unitarities first. Such an understanding has only gradually developed in the case of special–relativistic field theories, and to my knowledge it has not been discussed in the case of quantum fields in curved space–time.

\(^{1}\)Throughout these papers, we use the conventional “relativistic Heisenberg” picture, in which the state vector is unchanged (except when reduction occurs) and the field operators evolve with time. Thus probability is automatically conserved. The problematic unitarity concept is unitary implementability of evolution. This is explained in a little more detail in section 2.
Consider for definiteness the case of quantum charged particles responding to an external, classical, electromagnetic field. It is often asserted that, while there may be “intermediate” non-unitarities in this case (that is, if one only considers evolution to some intermediate time), they are not significant, because the $S$-matrix is unitary.

This position is indeed tenable if all one is interested in is the $S$-matrix, and only in those cases when it does turn out to be unitary — typically scattering through a potential which is turned on and off in finite time. But if one is interested in the intermediate regime, this is not a satisfactory position. When we come to quantum fields in curved space–time, we almost never “switch on and off” the gravitational field in finite time, so we must face the intermediate regime.\footnote{Also the position is not satisfactory for investigations of quantum measurement issues, where one wishes to take into account the facts that observers investigate only finite volumes of space–time, and that different observers can never synchronize their frames perfectly. The unitarity of the $S$-matrix only applies to evolution from one complete $t =$ constant surface in Minkowski space to another $t' =$ constant one, where both $t$ and $t'$ are inertial coordinates. Thus if data are taken over a surface by several observers who have uncertainties in synchronizing their clocks, the unitarity fails (Helfer 1996).}

What happens in this intermediate regime? In special-relativistic quantum field theories, presumably the non–unitarity results from neglecting fluctuations in the external potential; when these fluctuations are included, the evolution is supposed to be unitary.\footnote{Of course, we do not know that the evolution really is unitary, because we can only treat this theory — full, nonlinear, quantum electrodynamics in the case of charged particles and electromagnetic fields — perturbatively. Serious workers have occasionally suggested dropping the unitarity requirement as a way of evading the conclusions of Haag’s theorem.}

This is indeed a plausible picture, and if correct explains away the non-unitarities in special-relativistic problems. Since as we shall see in these papers, the non-unitarities are closely linked to the unboundedness–below, it is also plausible (but not a foregone conclusion) that accounting for the fluctuations will semi-bound the Hamiltonians.

However, there is more to the story. In order to understand this, recall that for linear field theories the non-unitarities are determined by when the Bogoliubov coefficients fail to satisfy a square-summability condition. In the most general situations, the sum involved may diverge because of: (a) infrared problems; (b) ultraviolet problems; (c) resonance phenomena assigning divergent weights to moderate modes. In what follows, I shall only consider ultraviolet divergences, but similar comments could be made for the other cases.

If the evolution fails to be unitarily implementable on account of ultraviolet divergences, then, with any finite ultraviolet cutoff $\Lambda$, the evolution is in fact unitarily implementable. What does this mean physically?

The answer to this can be found by examining the formulae for the quantum evolution operators in terms of the Bogoliubov transformations (e.g., in section \textsection 5 below). Details of this will appear elsewhere; here I shall only indicate the results. One examines how the evolution operator $U_\Lambda$ varies with the cutoff $\Lambda$, in particular, how $U_\Lambda$ affects modes of different frequencies. One finds that there is a critical scale $\Lambda_0$ which can be estimated in terms correlations of the external potential. For $\Lambda \ll \Lambda_0$, the operator $U_\Lambda$ varies smoothly with $\Lambda$. For $\Lambda \gg \Lambda_0$, the restriction of $U_\Lambda$ to the low-frequency sector has a reasonably well-defined limit; however, the action on high-frequency modes varies essentially chaotically (in a loose sense) as $\Lambda$ is increased.

What this means is that, in the cut-off theory but for $\Lambda \gg \Lambda_0$, qualitatively new features appear in the evolution. While these are not, strictly speaking, non-unitarities, they are certainly interesting.

At the moment, it is not known whether this “chaotic” behavior actually occurs in
any physically realizable situations. If there is a scale $\Lambda_{\text{fluct}}$ at which fluctuations in the external field must be accounted for, then the question is whether $\Lambda_0$ can exceed $\Lambda_{\text{fluct}}$. If not, then the fluctuations in the field become the dominant feature before the chaotic regime can be reached; on the other hand, if it is possible to have $\Lambda_0 < \Lambda_{\text{fluct}}$, then there can be a regime $\Lambda_0 < \Lambda < \Lambda_{\text{fluct}}$ in which effectively chaotic behavior occurs before the external-field approximation must be superseded. It may be that as a matter of principle this last possibility is excluded, but at the moment this remains an open question. It seems most likely that insight will be gained by investigating specific physical models.

The Unitarity Problem for Quantum Fields in Curved Space–Time  But the most important application of the present analysis of intermediate non-unitarity is to quantum fields in curved space–time. In this case, it is the gravitational field which is the external potential. If a picture like that expected for special-relativistic theories applies, then unitarity is restored by fluctuations in the gravitational field. It should be possible to build on the present analysis to make precise statements about what the characters of these fluctuations must be. In other words, we may be able to use the present work to deduce quantum characteristics of the gravitational field, assuming unitarity still holds in that context. It should be emphasized that these issues arise at moderate scales, far below the Planck threshold. Thus we have a new line of attack on quantum gravity, one which does not require hypotheses about the strong-gravity, Planck-scale, regime.

Relation to Algebraic Approaches  It has been recognized for a long time that it is useful to regard quantum field theory as constructed in two stages. First, one describes precisely an algebra $A$ of observables; then, one seeks a representation of this algebra on a physically acceptable Hilbert space. Specifying the algebra $A$ is rather like specifying a group by giving its multiplication table; specifying the representation is realizing the observables as operators on a Hilbert space.

Generally, by an algebraic approach to quantum field theory, one means an approach which starts from and emphasizes the algebra $A$. The most extreme form of this approach would seek to describe physics entirely in terms of this algebra without the construction of a representation. More moderate approaches (which are common) do make use of representations, although these representations are analogs of density matrices rather than state vectors. (The present paper, which emphasizes the construction of satisfactory Hamiltonians acting on Hilbert spaces of state vectors, would not be considered an algebraic approach.) One can recast quantum field theory in such algebraic terms, and then one has a formalism equivalent to the conventional one, and so it becomes a matter of taste or convenience which is to be preferred.

Algebraic approaches are attractive for some purposes, because they treat different representations with equal facility. In particular, when quantities which are singular in one representation may have sensible existences in other representations (such as the candidates for Hamiltonians in these papers), the algebraic approach can be a natural way of accommodating them. Indeed, the Hamiltonians have natural algebraic existences, because they are generators of symmetries of the field algebra $A$.

However, precisely this feature — the algebraic approach’s egalitarian treatment of different representations — can be a drawback. Precisely because of this, it is difficult or impossible to see, from the algebraic structure alone, how physically preferred representations (such as the ones of interest here) are distinguished.
While the results of these papers could be cast in terms of the algebraic approach, the papers’ goals are more naturally met in a conventional, representation-based, approach. While the present work is very mathematical, its goals are to provide enough structural background that it will be possible for subsequent work to develop a physical understanding of the significances of non-unitarities and ill-defined Hamiltonians. These are very much representation-based concerns, with the physically-dictated choices of representations playing a central role. Thus the representational approach seems to focus most directly on the physical issues.

I have emphasized that the point of the present papers is to lay a framework within which the significance of some potentially serious pathologies (non-unitarity, unboundedness-below of energy) can be analyzed, and I have argued that the representation-based approach is probably more suited to this than an algebraic one. On the other hand, once the physical significance of the pathologies is understood, one may have to reassess what the most appropriate formalism for the theory is. If, for example, it were to turn out that the pathologies were not of much physical significance, but only somehow mathematical niceties, then it could well be that the algebraic approach would be most useful, as a framework which can accommodate such behaviors without giving them undue weight.

The Hamiltonian

I shall now discuss the problematic nature of the Hamiltonian.

Of course, the Hamiltonian is simply the derivative of the evolution operator, so all of the comments above should apply, interpreted “infinitesimally,” to the Hamiltonian. However, to have such an interpretation, one needs an infinitesimal counterpart of the Bogoliubov–Shale criterion for unitary implementability, that is, a criterion for the existence of the Hamiltonian as a self-adjoint operator. Such criteria are provided in these papers. We may expect these criteria to be more practically useful, for many purposes, than that of Bogoliubov and Shale, since criteria in terms of the Hamiltonian do not require integration of the equations of motion.

Assuming the picture suggested above (of unitarity being saved by the breakdown of the validity of the external-field picture) for special-relativistic theories is correct, one would expect that the problems of ill-definition (as a self-adjoint operator) of the Hamiltonian are resolved by the same breakdown. Parallel to the question of the existence of an “effectively non-unitary regime,” one has the question of whether there is a sort of “effectively non-self-adjoint regime.” In other words, in a theory with cutoff \( \Lambda \), the Hamiltonian will depend sensitively on \( \Lambda \) for \( \Lambda \gg \Lambda_0 \). If \( \Lambda_0 \) is less than the scale \( \Lambda_{\text{fluct}} \) at which the external-field approximation breaks down, then one does have such a regime. Developments of the techniques of this paper should enable one to estimate \( \Lambda_0 \) in terms of the external field.

The foregoing applies to the Hamiltonian as the generator of evolution. However, there are important points beyond this. These have to do with the interpretation of the Hamiltonian as an energy operator, and with negative energies.

We wish to consider not just the total Hamiltonian, but the various energy operators that can be formed from the stress-energy, by integrating it against a smooth test field on a four-volume. Physically, these correspond to measurements of energy (or momentum, angular momentum, etc.) in finite spatial volumes with temporal averagings as well. These operators presumably are what figure in real experiments, since one can never measure a total (over all space) energy. The picture that emerges from these papers, as well as from previous work, is that (in the case of averaged energy operators), is that such averaged Hamiltonians exist as semi-bounded self-adjoint operators. But as the temporal extent of
the averaging is decreased: (a) the lower bounds diverge to $-\infty$; and (b) the Hilbert-space domains of the operators become more sparse, having only \{0\} as a limit.

It should be emphasized that this behavior occurs even in the simplest cases, for instance, for a Klein–Gordon field in Minkowski space (with no external potential). Consider for definiteness such a field, and an averaged energy operator
\[
\hat{H}(b, B) = \int \hat{T}_{\text{ren}}^{\text{ren}}(t, x, y, z) b(t) B(x, y, z) \, dt \, dx \, dy \, dz ,
\]  
where $b(t) \geq 0$, $B(x, y, z) \geq 0$ are smooth compactly-supported test functions effecting the temporal and spatial smearing of the energy density operator; we require
\[
\int b(t) \, dt = 1
\]  
to treat $b$ as an averaging. For any fixed $b, B$, the quantity $\hat{H}(b, B)$ is a self-adjoint operator, bounded below. But as the function $b$ becomes more sharply peaked at a given time, we find the conditions (a) and (b) of the previous paragraph. This means that there is no idealized operator
\[
\lim_{b(t) \to \delta(t)} \hat{H}(b, B)
\]  
representing the measure of the energy in a finite three-volume. In other words, “the energy in a spatial volume” is not a meaningful quantum observable. It is necessary to specify the scale of the temporal averaging in order to have a well-defined self-adjoint operator.

**Semiclassical Gravity** While many workers have recognized this point, it has not been taken fully to heart, I think, in an important area: attempts to understand the back-reaction of the quantum field on space–time. One would expect that this is determined by the energy density operator (and more generally by the components of the stress–energy), but we have just seen that this operator does not really exist; only averaged versions exist. This means that one must specify the scale of the averaging before one has a well-defined theory. In other words, the specification of the averaging scale is not just a technicality which will sort itself out; different scales give different theories, and one needs to know if it is possible to identify a physically plausible one for a given problem.

To be explicit, let us consider the most common starting-point for treatments of the back-reaction of the quantum field on space–time, the “semiclassical approximation:”
\[
R_{ab} - (1/2)Rg_{ab} = -8\pi G \left( T_{\text{ab}}^{\text{classical}} + \langle \hat{T}_{\text{ren}}^{\text{ren}} \rangle \right) .
\]  
This equation is a natural one to write down, but is it justified?

In general, one would expect such an approximation, where the quantum fields only couple through expectation values of an operator $\hat{O}$, to be valid when fluctuations in $\hat{O}$ are negligible. It is easy to construct examples, even in Newtonian gravity and non-relativistic quantum mechanics, in which this fails. Consider for instance two separated boxes, one at $r = a$ and the other at $r = -a$, and a particle of mass $m$ with probability $1/2$ of being in either box. Assuming the sizes of the boxes are negligible (compared to $\|a\|$), then the gravitational potential constructed from the expectation of the energy density is
\[
\frac{-Gm/2}{\|r - a\|} + \frac{Gm/2}{\|r + a\|} ,
\]
whereas the correct potential is presumably a quantum superposition

$$\frac{1}{\sqrt{2}} \left( \frac{Gm}{|r-a|} \right) + \frac{1}{\sqrt{2}} \left( \frac{Gm}{|r+a|} \right). \quad (7)$$

These two states of the gravitational field — (6) and (7) — are different, and that difference is in principle detectable in many ways. For example, an observer near one box experiences a certain gravitational red-shift relative to infinity according to (6); according to (7) she experiences, with probability $1/2$, either a much smaller or an almost doubled red-shift.\(^4\)

What this example shows is that in principle it is quite possible for the semiclassical approximation to fail, even in mild circumstances. Whether this failure is significant or not depends on exactly what regime one hopes to apply the approximation to. It is presumably far beyond the state of present technology to detect the difference between (6) and (7) with a laboratory experiment — one would need to be able to measure very fine differences in red-shifts with apparatuses much smaller than the scale $2||a||$ of the separation of the position eigenstates.

In general, for any proposed application of the semiclassical approximation, in order to check its credibility one needs to: (a) estimate the fluctuations; (b) specify the accuracy to which space–time is supposed to be modeled; (c) specify the time for which that model is supposed to be valid, before the errors made in the approximation accumulate and become significant. In some circumstances, such as the non-relativistic example above, elementary estimates can quickly convince one that the approximation is valid for practical purposes. However in other circumstances this is may not be so obvious.

Let us return now to the case of quantum fields in curved space–time. It is not hard to show that as the temporal averaging tends to zero, the fluctuations in $\hat{O}$ (here $\hat{O}$ is a temporally-averaged $\hat{T}_{ab}$) not only dominate the expectation value but actually diverge for all Hadamard states.\(^5\) This clearly raises questions about the validity of the semiclassical approximation. It is presumably possible to answer these in many cases; it is not possible to ignore the questions.

The divergent fluctuations of $\hat{T}_{ab}$ mean that equation (5) is not credible if interpreted literally. The equation might be valid if the right-hand side were replaced by some sort of temporal (or space–time) average of the expectation of the stress–energy. This indeed is presumably what happens in most everyday circumstances, where the quantum character of the matter is negligible for the purposes of understanding its effect on space–time. However, the main interest of quantum field theory in curved space–time attaches to those situations in which the quantum character of the fields is important. In those circumstances it becomes problematic to justify an equation like (5), even with a re-interpreted right-hand side. To do this, one would have to spell out the accuracy to which one wanted to model space–time classically, the time for which that model should hold, and the scale of the averaging. One would have to justify physically the averaging procedure. These sorts of questions have been very little investigated (see however Flanagan and Wald 1996 and Ford and Wu 1999).

Whether the semiclassical approximation turns out to be valid for a given purpose or not, careful attempts at its justification will deepen our understanding of the physics of the

\(^4\)While the argument in this paragraph has been deliberately phrased to make it as homely and unprovocative as possible, it implicitly involves quantum–gravitational assumptions. For example, the notion that the potential can be in a superposition of states implies that the potential must really be a quantum observable.

\(^5\)This follows from results in Helfer (1996). In terms of the notation of equation (8), below, the fluctuations contain a term $C_{\alpha\beta}C^{\alpha\beta}$, which diverges.
situation, as we ask exactly what scales are important, and how do we expect the behavior of the field to affect the space–time. And certainly the most interesting cases would be those for which (5) did not hold, even with a re-interpreted right-hand side. In such cases one would have to take into account the quantum character of the gravitational field. It is quite possible that such situations do exist: above, we saw that it seems necessary to include quantum fluctuations in the gravitational field in order to restore the unitarity of the field theory.

**Negative Energies** Much of the interest in these quantum stress-energies is on account of the prediction of relativistic quantum field theories that the renormalized, temporally averaged, energy densities can be negative. Thus if these stress-energies can be used as sources for Einstein’s equation, one has a violation of the Weak Energy Hypothesis, a key assumption underlying some of the most important results in classical relativity (the singularity theorems and the Area Theorem). Thus the understanding of precisely what sense the energy densities can be negative is a key problem, on whose resolution depend basic qualitative aspects of the behavior of space–time.

We must bear in mind that at present there is no direct experimental evidence of negative energy densities. Thus the importance of having as complete a theoretical understanding of these as possible.

**Formal Structures** To explain the foregoing more quantitatively, let us begin by writing down the formal expression for a Hamiltonian operator for a linear theory:

$$\hat{H} = C^{\alpha\beta}\hat{a}_\alpha\hat{a}_\beta + B^{\alpha\beta}\hat{a}^{*\beta}\hat{a}_\alpha + C_{\alpha\beta}\hat{a}^{*\alpha}\hat{a}^{*\beta} + \text{c-number term}. \quad (8)$$

Here $\hat{a}$, $\hat{a}^*$ are annihilation and creation operators, and $B^{\alpha\beta}$, $C^{\alpha\beta}$ are coefficients (self-adjoint and symmetric, respectively). If $C^{\alpha\beta} = 0$ and $B^{\alpha\beta}$ is self-adjoint, then the definition of the Hamiltonian is unproblematic; one has a structure much like that of the Hamiltonian for a free Klein–Gordon field in Minkowski space. However, if this situation is perturbed even slightly, difficulties may appear. For example, it is easy to see that the vacuum $|0\rangle$ cannot be in the domain of $\hat{H}$ unless $C^{\alpha\beta}\bar{C}_{\alpha\beta} < \infty$. This condition can very well be violated, even if the $C^{\alpha\beta}$ are uniformly small.

More severe problems may occur. It may be impossible to find any normalizable states on which $\hat{H}$ is well-defined. This means that $\hat{H}$ can have only a very limited existence, and certainly cannot be the self-adjoint operator that quantum theory requires an observable to be. These sorts of difficulties are potentially very serious, as they raise the

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6The measurement of the Casimir force is sometimes cited as such evidence, but that is a measurement of one of the “pressure” components of the stress–energy, not the energy density. There is only an indirect link between the two operators. Moreover, there are two sorts of concerns about the usual prediction of negative energy density between the plates of the Casimir apparatus. The first is that the plates have been unphysically idealized as perfect conductors; rough estimates show that for real plates there could be a separation-independent positive contribution to the energy density overwhelming the usual negative energy density (Helfer and Lang 1999); this would not alter the predicted Casimir force. Second, there may be difficulties of quantum measurement theory in meaningfully ascribing a negative energy density to the region between the plates (Helfer 1998).

7The modes annihilated and created by $\hat{a}$, $\hat{a}^*$ need not be particle modes; this will be discussed further, below. Also, the formal Hamiltonian (8) has been written in normal-ordered form. This is for purposes of orientation only. In the analysis that follows, criteria are developed for determining whether the quantum Hamiltonian exists without prior assumptions about what renormalization scheme is to be used. The second paper in this series will contain some further results, about when normal-ordering is adequate to define the theory.
question of what the operator character of the Hamiltonian, and hence of the dynamics, is. This should be contrasted with somewhat finer issues of renormalization which go to the kinematic question of what the c-number contribution to $\hat{H}$ is, for example, the computation of Casimir or ground-state energies. Those finer issues presumably cannot even be addressed until the operator character is properly understood.

We have seen that difficulties are potentially present when $C^{\alpha\beta} \neq 0$. Physically, this indicates that evolution by the Hamiltonian does not preserve the decomposition of the field into creation and annihilation parts. This situation occurs naturally in many settings. Most obviously, it is the situation in time-dependent external potential problems. In particular, it is the generic case for quantum fields in curved space–time. However, it can also occur when there is no explicit time dependence in the theory. If one has several linearly coupled fields, for example, in general one has $C^{\alpha\beta} \neq 0$; cases of current interest are the models for the quantum electromagnetic field in dispersive dielectric media (see, e.g., Barnett 1997). And the theory of squeezing revolves precisely around Hamiltonians with $C^{\alpha\beta} \neq 0$ (Loudon and Knight 1987).

Nature of the Present Paper

The main theorems to be given here have characters similar to some basic results in quantum theory, in that their general physical content can be appreciated without pursuing the analytic technicalities of their proofs. (Thus for example, physicists use daily spectral resolutions of self-adjoint operators without worrying about how the existence of such resolutions is proved; and one can appreciate the sense of the Stone–von Neumann theorem, that canonical quantizations of mechanical systems with finitely many degrees of freedom are unitarily equivalent, without examining its proof.) I have written these papers so as to confine the analytic technicalities to the proofs. I hope that the statements of the theorems will be accessible to general workers in quantum field theory.

There has been some previous work in this area. As mentioned earlier, Shale (1962) found the condition for a finite evolution to be unitarily implementable. Analyses parallel to Shale’s are central to the theory of loop groups, and it is possible that the present results may have analogs of interest there. Klein (1973) investigated the case of Hamiltonians, and provided a host of counterexamples to natural conjectures. More recently, Honegger & Rieckers (1996) established some results under fairly strong hypotheses on $C^{\alpha\beta}$.

The plan of the paper is this. The next section contains a brief discussion of the concept of unitary implementability. This can be skipped by those who understand the distinction between this sort of unitarity and that governing the state vector. Section 4 contains preliminaries, mainly the basic definitions needed to state the problem mathematically. Section 5 proves one of the two main theorems (Theorem 2), characterizing which classical Hamiltonian vector fields give rise to one-parameter unitary groups on the physical Hilbert space. In Section 6 (Theorem 3), it is shown that each group that arises in this way is automatically strongly continuous, and so possesses a self-adjoint generator, that is, a quantum Hamiltonian. Section 7 gives as an example the case of quantum fields in curved space–time; it is shown (Theorem 4) that evolution along the timelike unit normal to a Cauchy surface is not self-adjointly implementable unless the second fundamental form of the surface vanishes identically. Section 7 contains some comments.

The assumptions of the present paper are very general. In the next paper, I specialize to the case where the classical Hamiltonian functions are positive. Then one can say much more about the structure of the theory, and take up the question of whether the quantum Hamiltonians are bounded below. The third paper in the series will treat fermions.
Background. A good summary of the necessary quantum field theory, from the point of view of this paper, will be found in Wald’s (1994) book. The functional analysis can be found in Dunford and Schwartz (1958). In Section 5, I have made use of the theories of pseudodifferential and Fourier integral operators, for which see Treves (1980).

Summary of Notation. Here is a summary of the notation used. Unfortunately, there are quite a few things denoted conventionally by similar symbols.

- \( H \) is the space of solutions of the classical field equations, a real Hilbert space equipped with a symplectic form \( \omega \).
- \( H_C \) is the space \( H \) equipped with the complex structure defined by \( J \), and so made into a complex Hilbert space.
- \( \mathcal{H} \) is the physical Hilbert space of the quantum field theory, that is, the space on which the representation of the field algebra acts.
- \( \| \cdot \|_{\text{op}} \) is the operator norm.
- \( \| \cdot \|_{\text{HS}} \) is the Hilbert–Schmidt norm.
- \( A \) is the field algebra.
- \( A \) is the Hamiltonian vector field on the space of classical solutions.
- \( A \) is the Lie adjoint of \( A \), that is, the derivative of conjugation by \( g(t) = e^{tA} \).

Notes. Since \( H \) has no preferred inner product, I have usually been careful to emphasize the dependence of properties on \( J \). Thus one has \( J \)-symmetric transformations, etc. The Hilbert and Hilbert spaces used here are always assumed to be separable, that is, to have countable bases.

2 Unitary Implementability

The central question in this paper is, When does a group of motions on classical phase space have a unitary counterpart on Hilbert space? Since most of the quantum field-theoretic literature does not distinguish explicitly between this sort of unitarity and that governing the evolution of the state vector, it seems worthwhile to spell this out.

Let us consider a linear quantum field theory in the presence of a perhaps time-dependent external potential. This is constructed in two steps. First, one defines an algebra of fields \( \mathbb{A} \). These are not yet field operators, as they do not as yet operate on anything. Rather, the algebra \( \mathbb{A} \) is a mathematically precise way of expressing the canonical commutation relations which any such operators will be required to have. The second stage of the construction is the identification of the fields with specific operators on a Hilbert space, that is, the specification of a representation of the algebra \( \mathbb{A} \). (One can think of the steps as analogous to first defining a group by a multiplication table, and then giving a realization of it as a set of matrices acting on column-vectors.) In a linear field theory, the algebra \( \mathbb{A} \) is essentially determined by the classical phase space of the theory, since the canonical quantization specifies the commutation relations in terms of the Poisson brackets. There are in general many inequivalent representations one might choose for this algebra, and the question of which one is physically correct may be subtle.

For quantum fields in curved space–time, we accept the standard point of view, that the correct representation is a “Hadamard” one (cf. Wald 1994). This can be specified in various equivalent ways, for example, by demanding that on a dense set of states the leading short-distance asymptotics of the two-point functions agree with those in Minkowski space. However, it is only in section 6 that the details of the Hadamard form are used. Because the rest of this paper has a very general mathematical perspective, the conclusions
depend only on the fact that the physics does determine a representation. Thus most of the results are phrased in terms of compatibility issues between a generator of symmetries of $A$ (which we wish to implement as a quantum operator) and a representation; the precise way the representation is determined figures only in section 6. (The general class of representations we are concerned with are those given by symplectic quantization; explicit formulae are given in section 5.5.1. For particulars of the Hadamard representations, see Wald 1994; we also use formulae from Helfer 1996.)

In brief, then, besides the canonical commutation relations and the field equations, one needs an extra input to construct a quantum field theory: the choice of representation. In Minkowski space, in the absence of fixed external fields or boundary conditions which might break the relativistic invariance, one can find an essentially unique Poincaré-invariant representation, the Fock representation. However, in more general circumstances it can be a subtle issue to determine the physically correct representation. While we shall not need this here, it may be remarked that the choice of representation is encoded in the (infrared and ultraviolet) asymptotics of the two-point functions. Thus different representations may lead to different local quantum fluctuations, different vacuum polarizabilities, etc.

All representations considered here will have the same abstract mathematical form as the Fock representation in that they will be determined by a decomposition of the field operator into “creation” and “annihilation” parts, with a corresponding “vacuum” state. However, the modes created and annihilated may not correspond to particles, and may have no simple physical interpretations. Likewise, the “vacuum” state need not be interpretable as a physical vacuum. Such representations are adequate for almost all purposes, and more general ones can be constructed as direct sums or integrals of these.

By the evolution of the fields, we mean their change when the classical phase space is evolved along some Hamiltonian vector field, which in our case shall always respect the linear structure of the phase space. This evidently will determine an automorphism of the algebra $A$, and one would like to identify the generator of that automorphism with the quantum Hamiltonian. However, it may happen that the automorphism is not induced by any unitary motions of the physical Hilbert space. For a one-parameter group of motions, this means that the Hamiltonian cannot be realized as a self-adjoint operator. Two points should be emphasized about this sort of non-unitarity:

- The evolution in question is that of the algebra of fields, and not that of the state vectors. The state vectors do evolve unitarily — in fact, are unchanged in our Heisenberg picture (except when reduction occurs).

- The possibility of non-unitarily implementable evolution occurs only in quantum field theory. In quantum mechanics, when there are only finitely many degrees of freedom, the Stone–von Neumann Theorem guarantees that any two representations of the canonical commutation relations are unitarily equivalent. A corollary of this is that the Hamiltonians in the case of fields must always be formally self-adjoint, in a suitable sense. For any “coarse graining” of a quantum field theory to finitely many degrees of freedom will result in evolutions which are unitarily implementable. This means that the failure of unitary implementability, or of self-adjointness, must occur in the passage to the limit of infinitely many degrees of freedom.

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8 More precisely, the Hadamard condition determines a certain class, or “folium,” of representations.
9 And in any additional singularities the two-point functions may have, for example on account of boundary conditions.
3 Preliminaries

I shall begin by indicating, for the non-experts, the meanings of the objects in the symplectic treatment of the quantization of linear bose fields. Those familiar with this can skip to Section 2.2 to identify the terminology and symbols used in this paper.

3.1 Orientation

The usual Fock construction of free field theories in Minkowski space can be generalized to apply to linear fields responding to external potentials, in particular to fields in curved space–time. I shall summarize here how this is done.

Let $H$ be a real Hilbertable space, which in applications is the space of solutions (of a certain Sobolev regularity) to the classical field equations for a Bose field. This may be either in flat or curved space–time, and external fields may be present. We shall not explicitly discuss charged fields, but these can be treated with straightforward modifications of the present techniques. We require that there be given a symplectic form $\omega$ on $H$. Then $\omega$ determines an abstract algebra $\mathcal{A}$ of fields, obeying the canonical commutation relations. The term “abstract” is used here to emphasize that there has been as yet no construction of the quantum Hilbert space and representation of the algebra as operators on the space.

A particular representation (of the sort usually considered) of the field algebra is determined by choosing a positive complex structure, that is a map $J: H \to H$ which preserves $\omega$, satisfies $J^2 = -1$, and such that $\omega(v, Jv)$ is positive-definite. For free fields in Minkowski space, one chooses $J\phi = \pm i(\phi_+ - \phi_-)$, where $\phi_{\pm}$ are the positive- and negative-frequency parts of $\phi$. In Minkowski space, then, the positive-frequency fields are the $+i$ eigenspace of $J$, and from these the Fock representation is constructed in the usual way. The same mathematical prescription for constructing a representation of $\mathcal{A}$ works, however, for any positive complex structure $J$ on any Hilbertable symplectic space.

The choice of $J$ is physically important. Different choices of $J$ will generally lead to inequivalent representations of $\mathcal{A}$:

Theorem. (Shale 1962) Two positive complex structures, $J_1$ and $J_2$, lead to unitarily equivalent representations of $\mathcal{A}$ iff $J_1 - J_2$ is Hilbert–Schmidt.

(Recall that an operator $L$ is Hilbert–Schmidt if $\text{tr} L^*L < \infty$. Note that in finite dimensions, all operators are Hilbert–Schmidt.) It turns out that, at least for linear scalar fields in curved space–time, there is a natural choice of $J$, or more properly, an equivalence class of natural choices, in the above sense. These are characterized by having two-point functions whose leading short-distance behavior is the same as in Minkowski space (Wald 1994). Probably similar results are true for other field equations. In this paper, though, it will be unnecessary to examine how $J$ is determined; it will be a datum.

Since the representation will have the same mathematical structure as Fock space, we may speak of creation and annihilation operators. In general, these will have no simple interpretation in terms of particles, but refer to some other fundamental modes (whichever physical modes constitute the $+i$ eigenspace of $J$). We may also speak of a “vacuum” in

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10 A Hilbertable space is a topological vector space whose topological structure can be determined by an inner product, but without a preferred choice of inner product. The restriction to Hilbertable spaces is made to streamline some of the analysis, and could be weakened.

11 In the case of a gauge field, the following treatment applies to gauge equivalence classes of solutions.

12 This is a little bit of an oversimplification, as there may also be infrared effects.
this sense. In general this “vacuum” state has only mathematical interest, and does not have a physical interpretation as the vacuum. It will not be invariant under a change from one representation to a unitarily equivalent one.

Now if \( g : H \to H \) is a continuous linear map preserving \( \omega \), then \( g \) induces a change \( J \mapsto gJg^{-1} \), and so

**Corollary.** A symmetry \( g \) of \((H, \omega)\) is unitarily implementable on the representation determined by \( J \) iff \( J - gJg^{-1} \) is Hilbert–Schmidt.

This is simply the restatement, in the present formalism, of the well-known criterion for Bogoliubov transformations to be unitarily implementable.

Suppose now one has a one-parameter group \( g(t) \) of motions of \( H \) preserving \( \omega \). In most physical applications, this group is strongly continuous, meaning that for any fixed \( v \in H \), the function \( t \mapsto g(t)v \) is continuous. Under these circumstances, there is a generator \( A \) so that \( g(t) = e^{tA} \). In applications, this generator is typically a partial differential operator. For example, for evolution in time for the Klein–Gordon field, one has \( H = \{(\dot{\phi}, \phi)\} \) and

\[
A = \begin{bmatrix} 0 & 1 \\ \Delta - m^2 & 0 \end{bmatrix},
\]

where \( \Delta \) is the spatial Laplacian.

### 3.2 Definitions and Notation

Throughout, we shall let \( H_\mathbb{C} \) be a complex infinite-dimensional separable Hilbert space. The complex inner product on \( H_\mathbb{C} \) will be denoted \( \langle \cdot, \cdot \rangle \). We shall let \( H \) be the underlying real Hilbert space. Then we write \( J : H \to H \) for the real-linear map given by \( v \mapsto iv \), and

\[
\begin{align*}
(v, w) &= \Re(v, w) \\
\omega(v, w) &= \Im(v, w)
\end{align*}
\]

Then \( \langle \cdot, \cdot \rangle \) is the canonical real inner product on \( H \) and \( \omega \) is a symplectic form on \( H \) which is non-degenerate in that it defines isomorphisms from \( H \) to its dual. Note that

\[
(v, w) = \omega(v, Jw).
\]

Thus any two of \( \omega, J \) and \( \langle \cdot, \cdot \rangle \) determine the third.

Throughout, the real adjoint of a real-linear operator (perhaps only densely defined) \( L \) will be denoted \( L^r \). Thus the defining relation is \( \langle v, L^r w \rangle = \langle Lv, w \rangle \) with domain \( D(L^r) = \{ w \in H \mid \langle v, L^r w \rangle = \langle Lv, w \rangle \text{ for some } L^r w \text{ for all } v \in D(L) \} \). A useful result is the

**Proposition 1.** If \( g : H \to H \) is a continuous linear map preserving \( \omega \), then \( g \) is invertible and \( g^{-1} = -Jg^*J \). Conversely, the adjoint of \( g \) is \( g^* = -Jg^{-1}J \).

**Proof.** One has

\[
\omega(v, -Jg^*Jgw) = -(v, g^*Jgw) = -(gv, Jgw) = \omega(gv, gw) = \omega(v, w)
\]

for all \( v, w \in H \), and similarly

\[
(v, g^*w) = (gv, w) = \omega(gv, Jw) = \omega(v, g^{-1}Jw) = -(v, Jg^{-1}Jw).
\]

\( \Box \)
**Definition 1.** The symplectic group of $H$ is

$$\text{Sp}(H) = \{ g : H \to H \mid g \text{ is linear, continuous and preserves } \omega \}.$$  

Its elements are the symplectomorphisms.

The symplectic group does not depend on the real inner product on $H$ (or on the complex structure); it depends only on $\omega$ and the structure of $H$ as a Hilbertable space. It has naturally the structure of a Banach group, using the operator norm to define the topology.

**Definition 2.** The restricted symplectic group of $H_C$ is

$$\text{Sp}_{\text{rest}}(H_C) = \{ g \in \text{Sp}(H) \mid g^{-1}Jg - g \text{ is Hilbert–Schmidt} \}.$$  

That this set is closed under composition and inversion is a consequence of the fact that the Hilbert–Schmidt operators form an ideal. There is a natural topology on $\text{Sp}_{\text{rest}}(H_C)$; see Shale (1962). (We shall not need this topology here, since we shall be concerned exclusively with strong continuity.) Note that the complex-linear and -antilinear parts of $g$ are $g_\pm = (1/2)(g \mp JgJ)$. Thus $g^{-1}Jg - g$ is Hilbert–Schmidt iff $g_-$ is.

We recall that a strongly continuous one-parameter subgroup of $\text{Sp}(H)$ is a one-parameter subgroup $t \mapsto g(t)$ such that, for each $v \in H$, the map $t \mapsto g(t)v$ is continuous. (In general, one can also consider semigroups, defined for $t \geq 0$, but as every symplectomorphism is invertible, in our case every semigroup extends to a group, which is strongly continuous iff the semigroup is.) According to the Hille–Yoshida–Phillips Theorem, such groups have the form $g(t) = e^{tA}$, where $A$ is a densely-defined operator on $H$ (with certain spectral properties), and $\|g(t)\|_{\text{op}} \leq Me^{\epsilon |t|}$ for some $M, \epsilon \geq 0$. The spectrum of $A$ is confined to the strip $|\Re \lambda| \leq \epsilon$.

We now wish to consider the action of $g(t)$ by conjugation on certain operators. It is not difficult to see that, for any operator $L$ of finite rank, the function $t \mapsto g(t)Lg(-t)$ is continuous in Hilbert–Schmidt norm. Now suppose $L$ is a Hilbert–Schmidt operator. Then for any $\epsilon > 0$, we may write $L = L_\ell + L_\epsilon$, where $L_\ell$ has finite rank and $\|L_\epsilon\|_{\text{HS}} < \epsilon$. We then have

$$\|g(t)Lg(-t) - L\|_{\text{HS}} \leq \|g(t)L_\ell g(-t) - L_\ell\|_{\text{HS}} + \|g(t)L_\epsilon g(-t) - L_\epsilon\|_{\text{HS}}$$

$$\leq \|g(t)Lg(-t) - L_\ell\|_{\text{HS}} + (\|g(t)\|_{\text{op}}\|g(-t)\|_{\text{op}} + 1)\epsilon$$

(13)

(14)

We may make this less than any given $\eta > 0$, as follows. Assume first $|t| < 1$. Then the Hille–Yoshida–Phillips Theorem bounds $\|g(t)\|_{\text{op}}\|g(-t)\|_{\text{op}}$, and hence choosing $\epsilon$ we may make the second term as small as desired. Then the first term may be made small by restricting $|t| < \delta$. Thus conjugation by $g(t)$ is continuous at the identity on the Hilbert–Schmidt operators. But since conjugation is a group action, we have proved

**Proposition 2.** Let $g(t)$ be a strongly continuous one-parameter subgroup of $\text{Sp}(H)$. Conjugation by $g(t)$ induces a strongly-continuous one-parameter group $G(t) = e^{tA}$ on the space of Hilbert–Schmidt operators on $H$.

(The same proof would apply for the compact operators, or those of trace class.)
4 Characterization of Generators of $\text{Sp}_{\text{rest}}(H\mathbb{C})$

In this section, we shall prove the main theorem. We shall do this in two main stages. Our first goal is to find out what restrictions must be made on $A$ in order that $\exp tA$ be unitarily implementable for each $t$. We shall then show that no additional hypotheses need be made to ensure that these unitary maps can be chosen to form a strongly-continuous one-parameter group. Thus we shall be able to conclude that, when $\exp tA$ is implementable for each $t$, a Hamiltonian operator exists. This final argument is delicate, and I do not know of any reason a priori to expect the conclusion.

We begin by introducing a function measuring the change in complex structure: let

$$L(t) = g(t)Jg(-t) - J.$$  \hspace{1cm} (15)

The group law for $g(t)$ implies a “twisted” law

$$L(s + t) = g(s)L(t)g(-s) + L(s).$$  \hspace{1cm} (16)

If we formally differentiate this at $s = 0$, we find the differential equation

$$L'(t) = AL(t) - L(t)A + L'(0).$$  \hspace{1cm} (17)

Here

$$L'(0) = AJ - JA.$$  \hspace{1cm} (18)

The differential equation has the formal solution

$$L(t) = \int_0^t G(u)L'(0) \, du,$$  \hspace{1cm} (19)

where

$$G(t)Q = g(t)Qg(-t)$$  \hspace{1cm} (20)

for any operator $Q$.

We shall now show how these equations can be interpreted rigorously.

**Proposition 3.** $JA$ and $AJ$ are self-adjoint operators (on $H$ with the inner product $(\cdot, \cdot)$ defined in equation (11)) with domains $D(A)$ and $JD(A) = D(AJ)$, respectively.

**Proof.** We have

$$D((JA)^*) = \{v \in H \mid (JAw, v) = (w, (JA)^*v) \text{ for all } w \in D(JA)\}.$$  

Now, if $w \in D(A) = D(JA)$, we have

$$(JAw, v) = \partial_{t,0}\omega(Jg(t)w, Jv)$$

$$(JAw, v) = \partial_{t,0}\omega(w, g(-t)v)$$

$$= -\partial_{t,0}\omega(w, Jg(-t)v)$$

$$= \partial_{t,0}(w, Jg(t)v),$$

where $\partial_{t,0}$ means $\partial/\partial t$ evaluated at $t = 0$. The proof for $AJ$ is similar. \hfill $\square$
The condition $D(AJ) = D(JA)$ is the condition that $D(A)$ be invariant under $J$, that is, that the domain of $A$ be a complex space with complex structure $J$. This holds for all physical systems that have so far been studied, but there are at least mathematical examples for which it fails.

**Corollary 1.** The commutator $[A, J] = AJ - JA$ is naturally defined as a form

$$(v, [A, J]w) = (AJv, w) - (v, JAw)$$

on $D(AJ) \times D(A)$ (or on $D(A) \times D(AJ)$). We have

$$(v, [A, J]w) = \partial_{t,0}(v, g(t)Jg(-t)w) = \partial_{t,0}(v, L(t)w)$$

in this case.

**Proof.** We have

$$(v, g(t)Jg(-t)w) = \omega(v, Jg(t)Jg(-t)w)$$

$$= -\omega(g(-t)Jv, Jg(-t)w)$$

$$= -(g(-t)Jv, g(-t)w)$$

For $w \in D(A)$, we may write $g(-t)w = w - tAw + o(t)$; similarly, the last line displayed above becomes

$$-(Jv - tAJv + o(t), w - tAw + o(t)) = -(Jv, w) + t(AJv, w) - t(Jv, AW) + o(t),$$

which has the desired derivative.

And similarly:

**Corollary 2.** The $J$-antilinear part of $A$,

$$A_+ = (1/2)(A + JAJ),$$

exists as a $J$-symmetric form with domain $D(A)$, and also with domain $JD(A)$. The $J$-linear part of $A$,

$$A_- = (1/2)(A - JAJ),$$

exists as a $J$-skew form on both of these domains.

We can now make sense of the integral formula for $L(t)$.

**Proposition 4.** The formal expression (19) for $L(t)$ is valid in the sense of forms on $JD(A) \times D(A)$. That is, for any $v \in JD(A)$ and $w \in D(A)$, one has

$$(v, L(t)w) = \int_0^t \{ (v, G(u)AJw) - (v, G(u)JAw) \} du.$$

**Proof.** This follows by integration by parts; one has only to note that the terms can be arranged so that this is sensible.
4.1 Regularity of the Complex Structure

We show here that the function $L(t)$, measuring the change in the complex structure, is continuous and of at most exponential growth.

**Theorem 1.** If $g(t)$ is a strongly continuous one-parameter family of restricted symplectic transformations, then the function $t \mapsto L(t)$ is continuous (in the Hilbert-Schmidt norm).

**Proof.** We shall first show that the function is measurable. Let $\epsilon$ be a positive real number and $L_0$ a fixed Hilbert–Schmidt operator. The inverse image of the ball of radius $\epsilon$ at $L_0$ is
\[
\{ t \mid \sum_j \| (L(t) - L_0)e_j\|^2_H < \epsilon^2 \},
\]
where $e_j$ form an orthonormal basis for $H$. But the sum is a pointwise-convergent sum of non-negative continuous functions, hence lower semicontinuous, and hence measurable.

Now for positive integers $n$, consider the sets $\{ t \in (-1, 1) \mid \| L(t) \|_{HS} > n \}$. These form a decreasing sequence of sets of finite measure, with intersection $\emptyset$. Thus for large enough $n$ the set $S = \{ t \in (-1, 1) \mid \| L(t) \|_{HS} < n \}$ has positive measure. We may similarly find a set $T \subset (-1, 1)$, symmetric about the origin, of positive measure, and with $\| L(t) \|_{HS}$ bounded on $T$. However then the set $\{ t_1 + t_2 \mid t_1, t_2 \in T \}$ will contain an interval about the origin, and from the “twisted group law” and the Hille–Yoshida–Phillips Theorem we have
\[
\| L(t_1 + t_2) \|_{HS} \leq \| g(t_2) \|_{op}\| L(t_1) \|_{HS}\| g(-t_2) \|_{op} + \| L(t_2) \|_{HS}
\]
is bounded on this interval. Thus there exists an interval containing the origin on which $\| L(t) \|_{HS}$ is bounded.

We integrate the twisted group law in the form
\[
g(t)Jg(-t) - J = g(s + t)Jg(-s - t) - J + g(t)(g(s)Jg(-s) - J)g(-t)
\]
(for $t$ close enough to zero) over a closed interval $[s_0, s_1]$ near the origin:
\[
(s_1 - s_0)(g(t)Jg(-t) - J) = \int_{s_0}^{s_1} \left[ g(s + t)Jg(-s - t) - J \right] ds
\]
\[-g(t) \int_{s_0}^{s_1} \left[ g(s)Jg(-s) - J \right] ds g(-t)
\]
\[= \int_{s_0 + t}^{s_1 + t} \left[ g(u)Jg(-u) - J \right] du
\]
\[-g(t) \int_{s_0}^{s_1} \left[ g(s)Jg(-s) - J \right] ds g(-t)
\]
The first term of the last line tends to $\int_{s_0}^{s_1} [g(s)Jg(-s) - J] ds$ as $t \to 0$. The second term does, too, since we have shown that conjugation by $g(t)$ is strongly continuous on the Hilbert–Schmidt operators. Thus $L(t)$ is continuous at the origin.

Finally, at any value of $t$, for small enough $s$, we have
\[
\| L(t + s) - L(t) \|_{HS} = \| g(t)L(s)g(-t) \|_{HS} \leq \| g(t) \|_{op}\| L(s) \|_{HS}\| g(-t) \|_{op}
\]
which tends to zero as $s$ does.

\[\square\]
Proposition 5. For strongly continuous one-parameter families of restricted symplectic motions, one has

$$\|L(t)\|_{HS} \leq \alpha e^{\beta |t|}$$

for some \(\alpha, \beta \geq 0\). (If \(\|g(t)\|_{op} \leq Me^{c|t|}\), then one may choose any \(\beta > 2c\).)

Proof. A little algebra shows

$$L(nt) = [G((n-1)t) + G((n-2)t) + \cdots + 1]L(t).$$

From the Hille–Yoshida–Phillips Theorem, we know \(\|g(t)\|_{op} \leq Me^{c|t|}\) for some \(M \geq 1, c \geq 0\). Thus

$$\|L(nt)\|_{HS} \leq nM^2 e^{2c|nt|}\|L(t)\|_{HS}.$$  

For any \(\mu\) with \(|\mu| \geq 1\), write \(\mu = n + r\) where \(n\) is an integer and \(|r| < 1\), where \(r\) has the same sign as \(n\). Then we have

$$\|L(\mu)\|_{HS} = \|L(n(1 + r/n))\|_{HS} \leq nM^2 e^{2c|n|} \sup_{t \in (-2,1], \mu \in [1,2]} \|L(t)\|_{HS}$$

for \(|\mu| \geq 1\). The result now follows from elementary considerations.

We are now in a position to establish a useful property of unitarily implementable evolutions.

Proposition 6. Let \(A\) be the generator of a strongly continuous one-parameter subgroup of the restricted symplectic group. Then the \(J\)-antilinear part \(((\lambda - A)^{-1})_\_\) of its resolvent \((\lambda - A)^{-1}\) is Hilbert–Schmidt for the real part of \(\lambda\) sufficiently positive, and is \(o(\lambda)\) in the Hilbert–Schmidt topology as \(\lambda \to +\infty\).

Proof. Using a subscript minus to denote \(J\)-antilinear parts, we have

$$((\lambda - A)^{-1})_\_ = \int_0^\infty g_-(t)e^{-\lambda t} dt.$$  

A priori, this integral is known to exist only in the strong sense. However, it follows from the previous two results that \(g_-(t) = -(1/2)L(t)g(t)J\) is a locally integrable Hilbert Schmidt-valued function and that the integral converges for the real part of \(\lambda\) sufficiently positive. Multiplying by \(\lambda\), one easily shows that the resulting integral tends to \(g_-(0) = 0\) as \(\lambda \to +\infty\).

The converse of this fails; one can easily create counterexamples by considering direct sums of countably many two-dimensional symplectic spaces.

We close this subsection with some further properties of \(L\) and of operators derived from it, which will be useful in what follows.

Proposition 7. \(JL\) is a \(J\)-symmetric operator with spectrum strictly below unity.
Proof. We have
\[ JL = JgJg^{-1} + 1 = -(g^{-1})^*g^{-1} + 1 \]
where the asterisk denotes the real adjoint.

Now let us put
\[ g_\pm = (1/2)(g \mp JgJ) \]
for the \( J \)-linear and \( J \)-antilinear parts of \( g \). We have \( JL = 2g_+g_+^{-1} \), and hence \( g_+g_+^{-1} \) is a \( J \)-symmetric operator varying continuously in Hilbert–Schmidt norm, with spectrum bounded strictly below \( 1/2 \).

**Proposition 8.** For strongly continuous one-parameter families of restricted symplectic motions, the quantity \( gg_+^{-1} - 1 \) is a \( J \)-symmetric Hilbert–Schmidt operator, varying continuously with \( t \) in Hilbert–Schmidt norm.

Proof. We have
\[ gg_+^{-1} - 1 = (g_-g_-^{-1})[1 - g_-g_-^{-1}]^{-1}. \]
Since the first factor varies continuously in Hilbert–Schmidt norm and the second continuously in operator norm, the product varies continuously in Hilbert–Schmidt norm.

Note that \( JL(-t) = Jg^{-1}Jg + 1 = -2g^{-1}g_-J \), so \( g_-^{-1}g_- \) is also a continuous \( J \)-symmetric Hilbert–Schmidt operator, as is \( g_+^{-1}g - 1 \).

### 4.2 The Characterization Theorem

**Theorem 2.** A generator \( A \) of a strongly-continuous one-parameter subgroup of \( \text{Sp}(H) \) is a generator of a strongly-continuous one-parameter subgroup of \( \text{Sp}_{\text{rest}}(H_C) \) iff the following condition holds: Let \( g(t) = e^{tA} \), and let \( G(t) = e^{tA} \) be the associated one-parameter group acting on the compact operators on \( H \) by conjugation. Then for any \( \lambda \) in the resolvent set of \( A \), the quantity \( R(\lambda, A)L'(0) \) (is defined as a limit in the space of linear forms on \( D(AJ) \times D(A) \) and) is a Hilbert–Schmidt operator.

Proof. Note that \( D(AJ) \times D(A) \) is a Hilbertable space, and so will be the space of linear forms on it.

We have \( L(t) = \int_0^t G(u)L'(0) \, du \). The idea will be to integrate this against \( e^{-\lambda t} \). However, since \( L'(0) \) is only weakly defined, it will be easier to approach this integral as a limit. Consider then, for a Hilbert–Schmidt operator \( B \),
\[
\int_0^\infty e^{-\lambda t} \int_0^t G(u)B \, du \, dt = \int_0^\infty \lambda^{-1}e^{(A-\lambda)u}B \, du = -\lambda^{-1}R(\lambda, A)B
\]
Here the spectrum of \( A \) must lie in a strip \( |\Re z| < 2c \) for some \( c > 0 \), and so the integral converges for \( \lambda \) sufficiently positive. Now, as \( B \) approaches \( L'(0) \) (in the space of forms on \( D(AJ) \times D(A) \)), the left-hand side of this equation approaches \( \int_0^\infty e^{-\lambda t}L(t) \, dt \) in the space of forms, but this integral is in fact a Hilbert–Schmidt operator. (This follows from proposition[5].) Therefore, as \( B \) tends to \( L'(0) \) as a form, the quantity \( \lambda^{-1}R(\lambda, A)B \) tends to a limit, which we denote \( \lambda^{-1}R(\lambda, A)L'(0) \), equal to the integral.
For the converse, we note that
\[
\int_0^t G(u)L'(0)\,du = \lambda \int_0^t G(u)R(\lambda,A)L'(0)\,du + (1 - G(t))R(\lambda,A)L'(0),
\]
and the right-hand side is Hilbert–Schmidt in view of proposition 2.

This theorem is one of our main results. In applications, the operator \(A\) is the Hamiltonian operator for the classical field equations, acting on Cauchy data. The complex structure \(J\) is a pseudodifferential operator whose singular part is determined by the local structure of the field operator. Thus \(R(\lambda,A)L'(0)\) can be computed by pseudodifferential operator techniques from local data. Whether it exists as a Hilbert–Schmidt operator is in most cases easily read off simply by considering the orders of the dominant terms.

5 Existence of a Hamiltonian

The Characterization Theorem determines the conditions under which a strongly-continuous one-parameter subgroup of \(\operatorname{Sp}(H)\) lies in \(\operatorname{Sp}_{\operatorname{rest}}(H_C)\). In this case, it is what one might call pointwise unitarily implementable, that is, for each \(t\) there exists a unitary transformation \(U(t)\) on the Fock space implementing \(e^{itA}\). (Each of these transformations is determined uniquely up to phase.) One would like to know if (with an appropriate choice of phases) we have \(U(t) = e^{-i\hat{H}}\) for a self-adjoint Hamiltonian \(\hat{H}\). It turns out that this is always the case.

In order to prove this, and for its own interest, we shall work out an explicit formula for \(U(t)\). I would expect that formulas equivalent to this one (modulo phase) are known. However, it is worth going through the analysis explicitly here, for two reasons. First, the phase is of some interest and is technically difficult to analyze. Second, we need fine control over some of the terms in order to establish the strong continuity of \(U(t)\), and so a careful presentation is worthwhile.

5.1 The Representation

The representation (of the Weyl algebra of the field operators) is defined as follows. Let \(Z^a \in H_C\). (We shall use an index notation when convenient.) The \(Z^a\) will be creation operators, with \(\partial_a = \partial/\partial Z^a\) annihilation operators. Then the state wave functions are holomorphic functions \(\Psi(Z^a)\). It is sometimes convenient to distinguish between these wave functions and the abstract state vectors \(|\Psi\rangle\); the two are related by
\[
|\Psi\rangle = \Psi(Z^a)|0_Z\rangle,
\]
where \(|0_Z\rangle\) is the “vacuum” state. In this equation, the terms in the power series \(\Psi(Z^a)\) are thought of as creation operators.

The inner product is
\[
(\Psi|\Phi) = \int \overline{\Psi(\Phi)} e^{-(Z,Z)} DZ D\overline{Z}.
\]
This integral is defined as the integral of \(\overline{\Psi} \Phi\) against a promeasure; alternatively, it may be regarded as a short-hand for the power series in the coefficients of \(\Psi\). \(\Phi\) it formally determines. The normalization is fixed so that the norm of \(\Phi(Z) = 1\) is unity.
Now let $g = g(t)$ be a symplectomorphism. It induces an action on the field operators which is conventionally written as

$$Z'^a = \alpha^b Z^b + \beta^{ab} \partial_b$$  \hfill (27)  
$$\partial'_a = \delta^b_a \partial_b + \beta_{ab} Z^b.$$  \hfill (28)  

Here $\alpha, \beta$ are essentially the $J$-linear and -antilinear parts of $g(t)$, and are known as Bogoliubov coefficients. That $g(t)$ be a symplectomorphism is equivalent to

$$0 = \beta_{ac} \alpha^b c - \beta_{bc} \alpha^a c.$$  \hfill (29)  
$$\delta^a_b = \alpha^b c \alpha^a c - \beta_{bc} \beta^{ac}.$$  \hfill (30)  

Note that this implies $\alpha$ is invertible. That $g(t)$ lie in $\text{Sp}_{\text{rest}}$ is equivalent to requiring $\beta$ to be Hilbert–Schmidt.

The image of the vacuum is determined by the requirement that it be annihilated by all operators $\partial'_a$, and from this one finds the state is

$$N \exp -\frac{1}{2} Q_{ab} Z^a Z^b$$  \hfill (31)  

(or more precisely $N \exp -\frac{1}{2} Q_{ab} Z^a Z^b |0_Z\rangle$), where

$$Q_{ab} = (\tau^{-1})_a^b \beta_{cb}$$  \hfill (32)  

is symmetric and the normalization $N$ has modulus

$$|N| = |\det (\delta_{ab} - \overline{Q}_{ac} Q_{bc})|^{1/2}.$$  \hfill (33)  

The conditions on $\alpha$ and $\beta$ above imply that this state is well-defined (and that $|N|$, as defined here, is positive).

The evolution of a general state vector may now be determined. Let is write the abstract ket as

$$|\Psi\rangle = \Psi(z)|0_Z\rangle = \Psi'(Z')|0_{Z'}\rangle,$$  \hfill (34)  

where

$$|0_Z\rangle, \quad |0_{Z'}\rangle = N \exp -(1/2) Q_{ab} Z^a Z^b |0_Z\rangle$$  \hfill (35)  

are the vacua with respect to $J$ and $g(t^* J g(-t))$. Now write, in matrix notation,

$$Z' = \alpha Z + \beta \partial = \alpha Z + (\alpha \beta^T) \partial_{\alpha Z} = e^{\frac{1}{2} \alpha \beta^T \partial_{\alpha Z} \partial_{\alpha Z}} \alpha Z e^{-(1/2) \alpha \beta^T \partial_{\alpha Z} \partial_{\alpha Z}}.$$  \hfill (36)  

where $\partial_{\alpha Z} = \partial/\partial(\alpha Z)$. (Here we have used the relations $\partial/\partial(\alpha Z) = \alpha^{-1} T_\partial Z$ and $\alpha \beta^T = \beta \alpha^T$.) The last line of the displayed equation is valid, for example, as an operator identity with the exponentials defined by their formal power series, acting on polynomials, and extends by linearity to suitable holomorphic functions. Then we have

$$\Psi(Z) = \Psi'(Z') N e^{-(1/2) Q_{ab} Z^a Z^b}$$  \hfill (37)  

$$= e^{\frac{1}{2} \alpha \beta^T \partial_{\alpha Z} \partial_{\alpha Z}} \Psi'(\alpha Z) e^{-(1/2) \alpha \beta^T \partial_{\alpha Z} \partial_{\alpha Z}} N e^{-(1/2) Q_{ab} Z^a Z^b}.$$  \hfill (38)  

This formula defines $U(t)$, modulo phase. We know that it is a one-parameter projective unitary group. If we can show that this projective group is strongly continuous, and that the phases can be chosen to make the full group strongly continuous, then we shall be assured of the existence of a self-adjoint generator.
5.2 Continuity of Some Operations

**Proposition 9.** $Q_{ab}$ is a continuous function of $t$ in the Hilbert–Schmidt norm.

**Proof.** We shall work with $\overline{Q}^{ab}$, to avoid conjugating $\alpha$ and $\beta$.

For this, we must derive the precise relation between the $\alpha$’s, $\beta$’s, and $g$. This arises from the canonical quantization prescription, which in our case amounts to the replacement of the variables $Z^a, \bar{Z}_a$ with the operators $Z^a, \partial_a$. We see that $\alpha$ is precisely $g_+$, the $J$-linear part of $g$. We can work out $\beta$ from the identity

$$V_a Z'_a = V_a \alpha^a_1 Z^b + \beta^{ab} \bar{V}_a Z_b$$

from which we find

$$\beta^{ab} \bar{V}_a Z_b = \langle V, gZ \rangle - \langle Z, g_+ Z \rangle = \langle V, g_+ Z \rangle$$

and thus

$$\alpha^{-1} \beta^{bc} \bar{Z}_a Z_c = \langle Z, (g_+)^{-1} g_- Z \rangle.$$ 

It was shown in proposition 8 (and the comments following that proposition) that $(g_+)^{-1} g_-$ is continuous in Hilbert–Schmidt norm.

\[\Box\]

**Proposition 10.** With the choice of phase $N = |N|$, the image of the $J$-vacuum varies continuously with $t$.

**Proof.** Let $|\Psi_t\rangle$ be the image of the vacuum at time $t$. Then

$$\langle \Psi_t - \Psi_s | \Psi_t - \Psi_s \rangle = \int |N_t \exp(-(1/2)Q_{tab} Z^a Z^b - N_s \exp(-(1/2)Q_{sab} Z^a Z^b)|^2 \times e^{-(Z,Z)} DZ D\bar{Z}$$

$$= 2 - 2N_s N_t \Re \det(I - \overline{Q}_t Q_t)^{-1}.$$ 

Since $Q$ varies continuously in Hilbert–Schmidt norm, for any fixed $t$, this can be made as close to zero as desired by choosing $s$ close enough to $t$.

\[\Box\]

We now turn to a similar, more general computation. The trigonometric polynomials are dense in $\mathcal{H}$. (This is the present formulation of the well-known statement that the vacuum is a cyclic state for this representation.) We shall show that they vary continuously with $t$.

**Proposition 11.** With the choice of phase $N = |N|$, the image of any trigonometric polynomial varies continuously with $t$.

**Proof.** It is enough to establish this for trigonometric monomials.

For any $A \in \mathcal{H}$, let $W(A) = \exp(i(A \cdot Z + A \cdot \theta))$ be the corresponding Weyl operator. Here $A^a$ is $A$ as an element of $\mathcal{H}_C$, and $\overline{A}_a = \overline{A^a}$ is its complex conjugate. Then a trigonometric monomial is (a constant times) $W(A)|0\rangle$ for some $A$. The image of this state at time $t$ is

$$W(g(t)A) N_t \exp(-(1/2)Q_{tab} Z^a Z^b = N_t \exp \left\{ -(1/2) (A_t, A_t) \right\}$$

$$+ (1/2)Q_{tab} A^a_t A^b_t - (1/2)Q_{lab} Z^a Z^b + i(\overline{A}_a - Q_{tab} A^b_t) Z^a \right\},$$

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where $A_t = g(t)A$. We find

$$
\langle \Psi_s | \Psi_t \rangle = N_t N_s \det \left( \delta_{ab} - Q_{tbc} Q_{sca} \right)^{-1} 
\times \exp(1/2) \left\{ -\langle A_s, A_s \rangle - \langle A_t, A_t \rangle + Q_{tab} A_t^a A_t^b + Q_{tab} A_t^a A_t^b \right\} 
\times \exp(1/2) \left[ \begin{array}{cc} \delta_{ab} & \overline{Q}_s^{ab} \\ Q_{tab} & \delta_{ab}^{ab} \end{array} \right]^{-1} \left[ \begin{array}{c} A_s^a \\ -Q_s^{ab} A_t^b \end{array} \right].
$$

Since, as $s$ approaches $t$, we have $A_s \to A_t$ and $Q_s$ to $Q_t$ in Hilbert–Schmidt norm, this tends to unity as $s \to t$.

5.3 Existence Theorem for the Hamiltonian

We are now in a position to prove the existence of the Hamiltonian.

**Theorem 3.** If $e^{tA}$ is a strongly-continuous one-parameter subgroup of $Sp_{rest}$, then there exists a self-adjoint operator $\hat{H}$ on Hilbert space, unique up to an additive constant, such that $U(t) = e^{i\hat{H}t}$ implements $e^{tA}$.

**Proof.** With the choice of phases $N = |N|$, we have a projective unitary representation $U(t)$. The cocycle representing its deviation from a true representation is $U(s)U(t)U(-s-t)$. This can be computed by lengthy but straightforward means. In matrix notation, we find it is

$$
\left( \det(I + T_s Q_s)(I - Q_{s+t} Q_s(I - Q_{s+t} Q_s)^{-1}) \right)^{1/2}.
$$

Here the quantity whose determinant is to be taken is of the form $I + T$, where $T$ varies continuously in trace norm in $s$ and $t$. From this it follows that the cocycle is continuous, and so a continuous choice of phase is possible, making $U(t)$ into a one-parameter unitary group. Let such a choice be made.

Finally, we must show that this group is strongly continuous. Since the phases vary continuously, it is enough to show that the original, projective representation is strongly continuous. While this could probably be done directly from the formula above, it is probably clearer to give an indirect argument.

In the previous subsection it was shown that $U(t)$ is strongly continuous on a dense family of states. (Recall that now the phase has been chosen so that $U(t)$ is a one–parameter unitary group.) For any such state $|\Psi\rangle$ and any $t$, the state $(1/t) \int_0^t U(u)|\Psi\rangle \, du$ is in the domain of $\partial_{t=0} U(t)$. It follows that $U(t)$ has a densely-defined generator, which, because $U(t)$ is unitary, must be self-adjoint.

There is an interesting consequence of the formulas above:

**Corollary 3.** We have

$$
\langle 0 | e^{it\hat{H}} | 0 \rangle \neq 0
$$

for every $t$. 

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This means that, for any linear unitarily implementable evolution, if the state is initially vacuum, at any later time a quantum measurement to determine the state will have a positive probability of finding vacuum. While this result would be trivial for the second quantization of a one-particle Hamiltonian, here the operator \( \hat{H} \) need not preserve particle number, but may create or destroy pairs of particles, as the terms with quadratic contributions in \( Z \) or \( \partial \) enter into the evolution.

We have shown that under certain conditions a self-adjoint Hamiltonian \( \hat{H} \) exists generating a one-parameter family \( U(t) \) of unitary transformations. In the course of this argument, we determined \( U(t) \) up to phase. It would be of interest to determine the phase. However, here I shall only indicate that the problem is essentially one of renormalization.

We recall from the proof of theorem \( \mathbb{K} \) that the cocycle \( U(s)U(t)U(-s-t) \) for the projective representation was given by

\[
\left( \det(I + Q_tQ_s)(I - Q_{s+t}Q_s(I - Q_{t+s}Q_t^{-1})) \right)^{1/2}.
\]  

(41)

After a little algebra, this can be rewritten as

\[
\left( \det \alpha_{s+t}^{-1}\alpha_s^{-1} \right)^{1/2}.
\]  

(42)

If the determinant of \( \alpha \) were known to exist and depend continuously on \( t \), it would be simple to factor this: the phase would simply be \( (\det C \alpha)^{1/2} \). However, the present hypotheses do not ensure that the determinant of \( \alpha \) is defined. (We only know that \( \alpha \) is the identity plus a Hilbert–Schmidt term, not a trace-class term.) Thus the isolation of the phase is more delicate. One can think of this as finding a renormalized definition of \( \det C \alpha \).

### 6 Scalar Fields in Curved Space–Time

These papers were motivated by problems which arose in the theory of quantum fields in curved space–time. In this section, we apply the theory to that case. In particular, we settle an outstanding question: Is the Hamiltonian for such fields self-adjointly implementable in generic circumstances?

There are already two sorts of evidence pointing to a negative answer (Helfer 1996). First, it is known that evolution in time by a finite motion is not unitarily implementable. One might think that in this case a self-adjoint family of Hamiltonians could not exist, for if it did one could integrate it to deduce a unitary evolution, which would be a contradiction. However, in the present, non-autonomous, situation, the domains of the Hamiltonians could be time-dependent, and so the integration might not be possible. Thus the non-unitary implementability of finite motions is not, in itself, enough to imply non-self-adjoint implementability of the Hamiltonian.

The second sort of evidence comes from the formal expression for the Hamiltonian. This formal expression is known not to have any Hadamard states in its domain.\(^\text{13}\) (Hadamard states are in a sense the nicest test states in curved space–time, and often one takes as axioms that certain operators should have well-defined actions on these states.)

---

\(^{13}\)I am using the term “Hadamard state” here to mean a state vector \( |\Psi\rangle \) in the Hadamard representation, rather than, as is more common, a linear functional on the field algebra. A more precise definition will be given in the next footnote, after more terminology has been developed.
While this is some indication of a pathological structure, it does not prove that the Hamiltonian fails to exist — the Hamiltonian could be defined on some recondite domain, or its formal expression, derived under the assumption of a certain renormalization prescription being valid, might be incorrect. Thus, the formal singularity of the Hamiltonian is also inconclusive.

We shall show however that these arguments do suggest the correct answer: the Hamiltonian is not self-adjointly implementable. These conclusions (and somewhat broader ones) could be deduced a bit more quickly from the results of the next paper, but we wish to illustrate how the general structure developed here applies.

The general set-up is the following. We consider a space–time \((M, g_{ab})\) which is oriented, time-oriented and globally hyperbolic. Global hyperbolicity ensures that relativistic field equations are well-posed, and is necessary to ensure that a quantum field theory can be constructed along conventional lines. (See Wald 1994 for an outline of the construction of the quantum field theory.) We shall also assume that the Cauchy surfaces are compact. This is only done for technical reasons (it rules out all infrared difficulties and ambiguities): the problems we shall uncover will be manifested in the local, ultraviolet, divergences of certain traces, and would be present in any Hadamard quantization, whether the Cauchy surfaces are compact or not.

The field equation is

\[
(\nabla_a \nabla^a + m^2)\phi = 0, \tag{43}
\]

and the symplectic form is \(\omega(\phi, \psi) = \int_{\Sigma} (\psi^* d\phi - \phi^* d\psi)\). Here \(\Sigma\) is any Cauchy surface.

The complex structure is determined from the Hadamard two-point function, and is a certain pseudodifferential operator. If we decompose the initial data for the field at \(\Sigma\) as \([\dot{\phi}, \phi]\), as usual, and choose normal coordinates (in terms of the induced metric) on \(\Sigma\), then one has for the symbol of \(J\)

\[
\begin{bmatrix}
\text{sym} \alpha & |\xi|^{-1} \\
-|\xi| & -\text{sym} \alpha
\end{bmatrix} + \begin{bmatrix}
O(|\xi|^{-2}) & O(|\xi|^{-3} \log |\xi|) \\
O(|\xi|^{-1} \log |\xi|) & O(|\xi|^{-2})
\end{bmatrix}, \tag{44}
\]

where

\[
2\text{sym} \alpha = \pi_a \xi^a |\xi|^{-1} - \pi_{ab} \xi_a \xi_b |\xi|^{-3}, \tag{45}
\]

with \(\xi\) the Fourier transform variable, its norm with respect to the three-metric on \(\Sigma\) is \(|\xi|\), and \(\pi_{ab}\) the second fundamental form of \(\Sigma\) (Helfer 1996). (This \(\alpha\) is not the same as the Bogoliubov coefficient.)\(^{14}\)

We shall consider, for simplicity, evolution along the unit timelike normal to \(\Sigma\). In this case, the operator \(A\) is

\[
\begin{bmatrix}
0 & 1 \\
-s^2 & 0
\end{bmatrix}, \tag{46}
\]

where we have put \(s = \sqrt{-\Delta + m^2}\), with \(\Delta\) the Laplacian on the surface. This operator is determined from the classical stress–energy

\[
T_{ab}^{\text{classical}} = \nabla_a \phi \nabla_b \phi - (1/2) \epsilon_{ab} \nabla_c \phi \nabla^c \phi \tag{47}
\]

\(^{14}\)Once the complex structure \(J\) has been fixed, and the representation constructed as in the previous section, the Hadamard states may be defined as follows. They are the results of applying polynomials of creation operators \(\omega(\psi, \phi_-)\) to the \(J\)-vacuum. Here the creation operator \(\phi_-\) is the \(J\)-negative frequency part of the field, and the test functions \(\psi\) are required to be smooth (with compactly supported Cauchy data — a requirement that is automatically fulfilled here). The more common notion of a Hadamard state as a linear functional on the field algebra essentially corresponds to a density matrix formed from our Hadamard states.
in the usual way.

It is convenient to make a change of basis to make $A$ diagonal. Accordingly, we shall put $\phi = \phi_+ + \phi_-$ and $\phi = -is(\phi_+ - \phi_-)$. Here $\phi_{\pm}$ are not the positive- and negative-frequency parts of $\phi$ (which are defined using $J$), but are the projections of $\phi$ onto the eigenspaces of $A$. Acting on $\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix}$, the operator $A$ is

$$A = \begin{bmatrix} -is & 0 \\ 0 & is \end{bmatrix},$$

and the symbol of $J$ is

$$\text{sym} J = \begin{bmatrix} -i \alpha & 0 \\ \alpha & i \end{bmatrix} + O(|\xi|^{-2} \log |\xi|).$$

From these equations, we may read off the symbol of $g(t)Jg(-t)$, as a Fourier integral operator:

$$\left[ -i \alpha \begin{array}{c} \text{sym} \alpha(x - \hat{\xi}t)e^{-2i|\xi|t} \\ \text{sym} \alpha(x + \hat{\xi}t)e^{2i|\xi|t} \end{array} \right],$$

where $\hat{\xi}$ is the unit vector in the direction $\xi$. One sees directly from this that $g(t)Jg(-t) - J$, for finite $t$, will generally be an operator of order $-1$, and so not Hilbert–Schmidt. This is a direct estimate of $g(t)Jg(-t) - J$; it is not necessary here to use the characterization theorem.

However, it is instructive to see the connection between this and the characterization theorem. For this we need to compute $Q = (\lambda - A)^{-1}AJ$. Thus one should solve $[A, J] = \lambda Q - [A, Q]$ for $Q$, which is a linear evolution equation for $Q$ along the vector field generating $A$. This is an autonomous system, because the coefficients $A$ and data $J$ are given (as operators on initial data) at $\Sigma$.

Integration of this system can be accomplished directly, or by more general formal means. We shall take advantage of the computation for $g(t)Jg(-t)$ we have already made. We have the identity

$$(\lambda - A)^{-1}AJ = \int_0^\infty e^{-\lambda t}e^{tA}AJ \, dt.$$  \hspace{1cm} (51)

Using the formula (51), we find $(\lambda - A)^{-1}AJ$ is

$$2i|\xi| \left[ \int_0^\infty \text{sym} \alpha(x + \hat{\xi}t)e^{-(\lambda - 2i|\xi|)t} \, dt - \int_0^\infty \text{sym} \alpha(x - \hat{\xi}t)e^{-(\lambda + 2i|\xi|)t} \, dt \right].$$  \hspace{1cm} (52)

For large enough real $\lambda$, the contributions from $\alpha$ occur in arbitrarily small neighborhoods of $t = 0$, and so the leading behavior (of the upper-right term, say) is

$$-2i|\xi|(|\text{sym} \alpha|)(\lambda + 2i|\xi|)^{-1}.$$  \hspace{1cm} (53)

The contribution of this term to the Hilbert–Schmidt norm is

$$(2\pi)^{-3} \int_{\Sigma} d\Sigma(x) \int_{|\xi| > 0} d^3\xi \frac{4|\xi|^2}{\lambda^2 + 4|\xi|^2} |\text{sym} \alpha|^2.$$  \hspace{1cm} (54)
We now do the angular part of the integral. Let us put sym $\alpha = \beta^{ab}\hat{\xi}_a\hat{\xi}_b/|\xi|$ (cf. equation (45)). Then the angular contribution to the expression (54) is (up to radially symmetric factors)

$$\int_{S^2} \beta^{ab}\beta^{cd}\hat{\xi}_a\hat{\xi}_b\hat{\xi}_c\hat{\xi}_d d^2\hat{\xi} = (4\pi/5)\beta^{ab}\beta^{cd}\eta_{(ab}\eta_{cd)}$$

(55)

$$= (4\pi/15)(\beta^a_a\beta^b_b + 2\beta^{ab}\beta_{ab}) ,$$

(56)

where $\eta_{ab}$ is the three-dimensional Euclidean metric and the parentheses on the subscripts indicate symmetrization. This is a positive-definite symmetric form in $\beta^{ab}$, and so is positive unless $\beta^{ab}$ vanishes identically, that is, unless sym $\alpha$ vanishes identically.

Turning to the radial integral, since $\alpha$ is of order $-1$, this is ultraviolet divergent unless $\alpha$ vanishes identically. Inspecting the form of sym $\alpha$ (equation 45), we see that this would require $\pi_{ab}$ to vanish identically. Thus we have proved:

**Theorem 4.** Let $(M, g_{ab})$ be an oriented, time-oriented, globally hyperbolic space–time with compact Cauchy surfaces. Consider the quantum field theory of a scalar field subject to the equation

$$(\nabla^a\nabla_a + m^2)\phi = 0$$

in a Hadamard representation. Let $\Sigma$ be a particular Cauchy surface, and $A$ the operator generating evolution along the unit normal determined by the usual classical stress–energy, equation (47). If the second fundamental form of $\Sigma$ does not vanish identically, then $A$ is not self-adjointly implementable.

In the set of Cauchy surfaces, those with vanishing second fundamental forms constitute a thin set in any reasonable topology. Indeed, the class of globally hyperbolic space–times admitting a Cauchy surface with vanishing second fundamental form is arguably a thin set in any reasonable topology. (In the case of zero classical stress–energy, these are space–times which possess time-reflection symmetry.) We may say that generically $A$ is not self-adjointly implementable.

More generally, one would conjecture that a Hamiltonian $A$ corresponding to evolution along a vector field $v^a$ at $\Sigma$ would not be self-adjointly implementable unless $v^a$ satisfied Killing’s equation (restricted to $\Sigma$) (cf. Helfer 1996, p. L133).

We close with a comment about the conformally coupled massless field

$$(\nabla_a\nabla^a + (1/6)R)\phi = 0$$

(57)

with its “new, improved” stress–energy

$$T^{\text{classical}}_{ab} = (2/3)\nabla_a\phi\nabla_b\phi - (1/6)g_{ab}\nabla_c\phi\nabla^c\phi - (1/3)\phi\nabla_a\nabla_b\phi$$

$$+ (1/18)R\phi^2 g_{ab} - (1/6)\phi^2 R_{ab} .$$

(58)

The field equation here agrees with that of the massless case of the ordinary scalar field in cases where $R = 0$; in particular, in Minkowski space. But the evolution of the field data as generated by the stress–energy is different, because the evolutions are determined by the Poisson brackets of the fields with the energy integrals $\int T_{ab}\xi^a d\Sigma^b$, and the different stress–energies yield different integrals. (One way of viewing this is that the “new, improved” stress–energy contains terms which correct the evolution of $\dot{\phi}$ to account for $\phi$ having conformal weight $-1$.)
One can analyze the conformally coupled field in a manner completely parallel to that for the ordinary scalar field. I shall not give the details of the computations here. One finds that the operator $A$ is then no longer given by equation (46), but has correction terms which are

$$
\begin{pmatrix}
0 & 0 \\
0 & -(2/3)\pi_a^a
\end{pmatrix} + \text{lower-order terms. (59)}
$$

These turn out to cancel the highest-order pure-trace contributions of $\pi_{ab}$ to $g(t)Jg(-t) - J$, and we wind up with

**Theorem 5.** Let $(M, g_{ab})$ be an oriented, time-oriented, globally hyperbolic space–time with compact Cauchy surfaces. Consider the quantum field theory of a conformally coupled scalar field (with field equation (57)) in a Hadamard representation. Let $\Sigma$ be a particular Cauchy surface, and $A$ the operator generating evolution along the unit normal determined by the “new, improved” stress–energy, equation (58). If the second fundamental form of $\Sigma$ is not pure trace, then $A$ is not self-adjointly implementable.

### 7 Comments

The results of this paper were outlined in the introduction, and no summary will be given here. Rather, this section contains a few technical comments.

The two main general results in this paper are Theorem 2 which establishes which classical Hamiltonian vector fields generate motions which are implementable on the quantum Hilbert space by unitary transformations, and Theorem 3 which shows that when such unitary implementation is possible a quantum Hamiltonian necessarily exists.

The latter result is gratifying physically, in that it means a certain type of pathology is absent. (The pathology would be that each classical canonical transformation in the one-parameter family would have a unitary implementation, but that it would not be possible to choose this family of unitary motions with strong enough continuity properties to guarantee the existence of a self-adjoint generator.) However, at least the present argument for this is rather delicate (one has “just enough” convergence to establish it). It would be worthwhile to find a simple argument to replace it.

In some sense, the lesson of Theorem 2 is that what is important is not so much the generator $A$ of the classical motions (that is, the Hamiltonian vector field), as its Lie adjoint $A^\dagger = [A, \cdot]$; one needs

$$
(A - \lambda)^{-1}AJ
$$

(60) to be Hilbert–Schmidt (for sufficiently large $\lambda$) in order that $A$ be self-adjointly implementable. If $A$ were known to have a spectral representation, then this criterion would amount to saying that, in terms of its spectral resolution, the quantity $AJ$ projected near the origin (that is, $\int_{|\lambda|<\alpha} dE(\lambda)AJ$, where $dE(\lambda)$ is the spectral measure) was Hilbert–Schmidt, and that $J$ projected near infinity was. In other words, the complex structure $J$ should have certain asymptotics in terms of the spectral resolution of $A$.

We shall see in the sequel that classically positive Hamiltonians have Hamiltonian vectors which are necessarily spectral operators (and hence $A$ is spectral). However, in more general circumstances, this need not be the case. For example, take the phase space to be the countable direct sum $\oplus_n \{(p_n, q_n) \in \mathbb{R}^2\}$ of two-dimensional phase spaces. The Hamiltonian function will be

$$
H = p_1q_2 + p_2q_3 + \cdots
$$

(61)
so that the induced canonical transformation is, in block form with respect to the \((q,p)\) decomposition

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & \cdots \\
& & & & \ddots \\
& & & & 0 & 0 & 0 & 0 & \cdots \\
& & & & -1 & 0 & 0 & 0 & \cdots \\
& & & & 0 & -1 & 0 & 0 & \cdots \\
\end{pmatrix}
\]

(blank places are occupied by zeroes). This decomposes into two shift operators, which are the well-known to be non-spectral (Dunford & Schwartz 1971). (We remark that this operator is not only bounded but contractive: \(\|Av\| \leq \|v\|\), where \(\|\cdot\|\) is the standard \(L_2\) norm.)

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