Refined Algebraic Quantization and Quantum Field Theory in Curved Space-Time

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Abstract

Application of the so-called refined algebraic quantization scheme for constrained systems to the relativistic particle provides an inner product that defines a unique Fock representation for a scalar field in curved space-time. The construction can be made rigorous for a general globally hyperbolic space-time, but the quasifree state so obtained turns out to be unphysical in general. We exhibit a closely related pair of Fock representations that is also defined generically and conforms to the notion of in- and outgoing states in those situations where particle creation by the external field is expected.
1 Introduction

In the early years of quantum field theory in curved space-time the two most important foundational problems were deemed to be the following: First, how to generalize the notion of vacuum in Minkowski space to space-times with a lesser degree of symmetries, and second, how to get rid of the divergencies that appear in the expectation value of the energy-momentum tensor and related objects of physical interest. After more than thirty years of development, which was most rapid in the years immediately following the discovery of the Hawking effect in 1974, a certain stage of maturity has been reached, and the following consensus regarding the above problems appears to have emerged. First, particle-like states may not exist in a generic space-time, and quantum field theory should be formulated in a manner that is not tied to a particular Fock representation, just as General Relativity does not require the use of a particular coordinate system. Second, a consistent regularization scheme exists for a large class of states called Hadamard states, and it has been proposed that there are no physical states outside this class.

In this paper, without questioning the answer to the first point raised above, we nonetheless would like to draw attention to the fact that there exist mathematically preferred states which are invariantly defined and have physical significance. This is completely analogous to the existence of preferred reference frames in General Relativity, e.g. free falling ones, that are more “physical” than others. We shall infer the existence of preferred states (which have been known for quite a long time) from the so-called refined algebraic quantization scheme of Ashtekar et al. [1] which has been devised in the context of the connection dynamics formulation of canonical quantum gravity, but will be applied here only to a very simple system, namely the relativistic particle. Although this application falls within relativistic quantum mechanics, not quantum field theory, it is straightforward to associate a unique Fock representation with it. This turns out to be unphysical in general, however. But a closely related pair of Fock representations appears to correspond exactly to the notions of in- and outgoing states in those situations where particle creation by the external field is expected. Moreover it is a characteristic of these states that they allow a simple description of particle creation within the framework of relativistic quantum mechanics after all.

It is our aim to present a mathematically rigorous construction of the various representations. Therefore some necessary preliminaries of quantum field theory in curved space-time are recapitulated in Sec. 2, and the nuclear spectral theorem plays a prominent role in the application of the refined algebraic quantization method given in Sec. 3. Physical considerations enter more directly in Sec. 4, but for the application of the formalism to concrete physical situations we have to refer to the published literature.

2 Linear scalar field in curved space-time

We begin with a review of the standard construction of quantum field theory in curved space-time as formulated by Kay and Wald [2, 3]. Let \((M, g_{ab})\) be a globally hyperbolic
space-time manifold. This implies that $M$ is a foliation of spacelike Cauchy hypersurfaces,

$$M = \bigcup_t \Sigma_t,$$  \hspace{1cm} (2.1)

when $t$ is a global time coordinate. We shall consider a scalar field $\phi$ on $M$ whose classical action is of the form

$$S[\phi] = \frac{1}{2} \int d^4x|g|^{1/2}(g^{ab}\nabla_a\phi\nabla_b\phi - V(x)\phi^2)$$  \hspace{1cm} (2.2)

$$\equiv \int dtL[\phi, \dot{\phi}]$$  \hspace{1cm} (2.3)

where the dot denotes differentiation with respect to $t$. Variation of the action gives rise to the classical field equation

$$\hat{C}\phi = 0$$  \hspace{1cm} (2.4)

$$\hat{C} := \hat{\square}_g + V$$  \hspace{1cm} (2.5)

$$\hat{\square}_g = g^{ab}\nabla_a\nabla_b = |g|^{-1/2}\partial_a|g|^{1/2}g^{ab}\partial_b.$$  \hspace{1cm} (2.6)

A popular choice for the “potential” $V$ is

$$V = \frac{1}{6}R + m^2$$  \hspace{1cm} (2.7)

implying conformal invariance for the massless field at the classical level. The Hamiltonian formalism for the field $\phi$ becomes most transparent upon a $3 + 1$ decomposition of the metric. In particular one introduces the induced Riemannian 3-metric on $\Sigma_t$, denoted by $h_{ij}$, and the future-directed unit normal vector field $n^a$ on $\Sigma_t$. Then the canonically conjugate momentum of $\phi$ may be expressed as

$$\Pi = \frac{\delta L}{\delta \dot{\phi}} = \frac{1}{2}|h|^{1/2}n^a\nabla_a\phi,$$  \hspace{1cm} (2.8)

$h$ denoting the determinant of $h_{ij}$. We define the phase space $\Gamma$ as

$$\Gamma = \{(\varphi, \pi) | \varphi, \pi \in C^\infty(\Sigma_0)\}.$$  \hspace{1cm} (2.9)

Because of global hyperbolicity we have

$$\Gamma \cong S$$  \hspace{1cm} (2.10)

where $S$ is the space of classical solutions of (1.4) with $C^\infty_0$ initial data. Moreover the linearity of the field equation implies $\Gamma \cong T_P\Gamma$ (the tangent space at an arbitrary point $P \in \Gamma$) so that the canonical 2-form defines a natural symplectic form $\Omega : S \times S \to \mathbb{R}$. It is given by

$$\Omega(\varphi_1, \varphi_2) = \int_{\Sigma_t} (\varphi_1\pi_2 - \pi_1\varphi_2)d^3x = \int_{\Sigma_t} \varphi_1 \nabla_a \varphi_2 d\sigma^a$$  \hspace{1cm} (2.11)
and clearly independent of $t$. (The hypersurface element is $d\sigma^a = n^a|h|^{1/2}d^3x$ in local coordinates on $\Sigma_t$.) Classical observables are functionals on $S$, i.e. maps from $S$ to $\mathbb{R}$. The physically most prominent one, the point field

$$\Phi(x) : \varphi \mapsto \varphi(x)$$

(2.12)
is a distribution, which becomes an operator-valued distribution upon quantization and is therefore not considered for constructive purposes. Instead, one considers the “symplectically smeared” fields

$$\Omega_\psi \equiv \Omega(\psi, \cdot) : \varphi \mapsto \Omega(\psi, \varphi).$$

(2.13)

(If one lifts the restriction of the solution space to $C^\infty_0$ initial data, then one has the following relations between the smeared and point fields: $\Phi(x) = \Omega_{G(\cdot, x)}; \Omega_\psi = \Omega(\psi, \Phi(\cdot))$, where $G$ denotes the fundamental solution or classical propagator.) We define the classical algebra of observables as the commutative algebra generated by the smeared fields. Its Poisson structure is implied by the canonical Poisson bracket:

$$\{\Omega_{\psi_1}, \Omega_{\psi_2}\} = \Omega(\psi_1, \psi_2).$$

(2.14)

Canonical quantization introduces a quantum algebra of observables with generators $\hat{\Omega}_\psi$ and the canonical commutation relations

$$[\hat{\Omega}_{\psi_1}, \hat{\Omega}_{\psi_2}] = i\Omega(\psi_1, \psi_2)\mathbf{1}$$

(2.15)

(we set $\hbar = 1$). States are positive normed linear functionals on this algebra. The physically most interesting states are defined in terms of Fock space constructions. A Fock space may be constructed in the following way: Select a space $S^{\mathbb{C}+}$ of complex solutions of (2.4) ($S^{\mathbb{C}+} \cap \overline{S^{\mathbb{C}+}} = \{0\}$) such that (i) there is a linear bijective map $P^+ : S \rightarrow S^{\mathbb{C}+}$ with $\varphi = P^+ \varphi + \overline{P^+ \varphi} \forall \varphi \in S$, (ii) $\Omega$ is extendible to $S^{\mathbb{C}+} \oplus \overline{S^{\mathbb{C}+}}$ and (iii) the charge form, defined by

$$(\psi_1, \psi_2) := i\Omega(\overline{\psi_1}, \psi_2)$$

(2.16)
is positive on $S^{\mathbb{C}+}$ and $(S^{\mathbb{C}+}, \overline{S^{\mathbb{C}+}}) = 0$. (Note that $S^{\mathbb{C}+}$ is not required to be a subspace of the complexification of $S$, $\mathbb{C} \otimes S$, the reason being that this would not yield a physical one-particle Hilbert space even in Minkowski space-time.) The one-particle Hilbert space $\mathcal{H}^+$ is defined as the completion of $S^{\mathbb{C}+}$ with respect to the charge form. It follows from (iii) that

$$(\cdot, \cdot)|_{\mathcal{H}^+} \geq 0$$

(2.17)

$$(\cdot, \cdot)|_{\overline{\mathcal{H}^+}} \leq 0$$

(2.18)

$$\langle \mathcal{H}^+, \mathcal{H}^+ \rangle = 0.$$  

(2.19)

(Eq. (2.18) is implied by $(\overline{\psi}, \psi) = -(\psi, \varphi)$.) From $\mathcal{H}^+$ we construct a representation $\rho$ of the algebra of observables in the Fock space

$$\mathcal{F}_s(\mathcal{H}^+) = \bigoplus_{n=0}^{\infty} \otimes_s^n \mathcal{H}^+$$

(2.20)
with
\[
\rho(\hat{A}_\varphi) = -ia(P^+\varphi) + ia^\dagger(P^+\varphi)
\] (2.21)
where \(a(\psi)\) and \(a^\dagger(\psi)\) are the standard annihilation and creation operators associated with \(\psi \in \mathcal{H}^+\) with commutator
\[
[a(\psi_1), a^\dagger(\psi_2)] = (\psi_1, \psi_2)1.
\] (2.22)

Obviously the whole construction depends on the choice of \(S_{C^+}\); different choices may yield unitarily inequivalent representations.

It turns out that any choice of \(S_{C^+}\) is characterized by a certain positive definite inner product on \(S\), and that this characterization provides a very useful reformulation of the above construction. In order to prepare this reformulation we observe that a positive inner product \(\langle \, , \rangle\) on \(S\) may be defined by
\[
\langle \psi_1, \psi_2 \rangle := 2\text{Re} \left( P^+\psi_1, P^+\psi_2 \right)
\] (2.23)
so that
\[
(P^+\psi_1, P^+\psi_2) = \frac{1}{2} \langle \psi_1, \psi_2 \rangle + \frac{i}{2} \Omega(\psi_1, \psi_2)
\] (2.24)
(the imaginary part of the expression appearing in (2.24) is independent of the choice of \(S_{C^+}\)). Using the Schwarz inequality for the charge form on \(S_{C^+}\),
\[
(\psi_1, \psi_1)^{1/2} (\psi_2, \psi_2)^{1/2} \geq |(\psi_1, \psi_2)| \geq |\text{Im}(\psi_1, \psi_2)|,
\] (2.25)
for \(\psi_i = P^+\varphi_i\) and noting that this chain of inequalities can be saturated, we deduce
\[
\langle \varphi_1, \varphi_1 \rangle = \sup_{\varphi_2 \neq 0} \frac{[\Omega(\varphi_1, \varphi_2)]^2}{\langle \varphi_2, \varphi_2 \rangle}.
\] (2.26)

The Fock construction may now be reformulated as follows. Let \(\langle \, , \rangle\) be a positive definite scalar product on \(S\) with the “supremum property” (2.26) relative to the charge form. Complete \(S\) with respect to \(\langle \, , \rangle\) to obtain a real Hilbert space \(\hat{S}\). Eq. (2.26) implies that \(\Omega : S \times S \to \mathbb{R}\) is bounded and by continuity extendible to \(\hat{S} \times \hat{S}\). Define \(J : \hat{S} \to \hat{S}\) by
\[
\Omega(\varphi_1, \varphi_2) = \langle \varphi_1, J\varphi_2 \rangle.
\] (2.27)

One verifies easily that \(J^\dagger = -J\), \(J^2 = -1\) (i.e. \(J\) defines a complex structure, but it will not be used in this sense). Next complexify \(\hat{S}\) to \(\hat{S}_C = \mathbb{C} \otimes \hat{S}\) and extend \(\Omega\) (bilinear), \(\langle \, , \rangle\) (sesquilinear) and \(J\) to \(\hat{S}_C\) by complex linearity. Define the complex Hilbert space \(\mathcal{H}^+\) as the eigenspace of \(J\) with
\[
J_{\mathcal{H}^+} = -i
\] (2.28)
and let \(\bar{P}^+\) be the orthogonal projection from \(\hat{S}_C\) on \(\mathcal{H}^+\). It can then be verified that \(\mathcal{H}^+\) has the properties of a one-particle Hilbert space. Moreover defining
\[
P^+ = \bar{P}^+|_S
\] (2.29)
we recover (2.24). Thus the choice of a complex solution space $S^{C^+}$ is indeed equivalent to the choice of a certain inner product $\langle \cdot , \cdot \rangle$ on $S$ with the property (2.26).

The above construction may be generalized to represent general quasifree states (of which the Fock vacua form only a subclass). These states are best introduced on the Weyl algebra $\mathcal{A}$, a subalgebra of the algebra of observables that is generated by the unitary elements

$$\hat{W}_\psi = e^{i\hat{\Omega}_\psi}.$$  

The canonical commutation relations (2.15) imply the Weyl relations

$$\hat{W}_\varphi_1 \hat{W}_\varphi_2 = e^{\frac{i}{2} \Omega(\varphi_1, \varphi_2)} \hat{W}_{\varphi_1+\varphi_2}.$$  

Let $\langle \cdot , \cdot \rangle : S \times S \to \mathbb{R}$ be positive with

$$\langle \varphi_1, \varphi_1 \rangle \langle \varphi_2, \varphi_2 \rangle \geq [\Omega(\varphi_1, \varphi_2)]^2.$$  

This inequality is a certain relaxation of the supremum condition (2.26) and will therefore yield a wider class of Fock space constructions than considered previously. The inner product $\langle \cdot , \cdot \rangle$ defines a quasifree state $\omega$ by

$$\omega(\hat{W}_\varphi) = e^{-\frac{1}{2} \langle \varphi, \varphi \rangle}.$$  

Any quasifree state (meaning a state whose truncated $n$-point functions vanish for $n > 2$) may be related to an inner product in this way, the inequality (2.32) ensuring the positivity of the state functional. Although $\hat{\Omega}_\varphi$ does not belong to the Weyl algebra, the “smeared two-point function” may be defined by

$$\langle \hat{\Omega}_{\varphi_1}, \hat{\Omega}_{\varphi_2} \rangle_\omega = -\frac{\partial^2}{\partial s \partial t} \left[ \omega(W_{s\psi_1+t\psi_2}) e^{is\Omega(\psi_1, \psi_2)/2} \right]_{s=t=0}$$  

and eq. (2.33) implies

$$\langle \hat{\Omega}_{\varphi_1}, \hat{\Omega}_{\varphi_2} \rangle_\omega = \frac{1}{2} \langle \varphi_1, \varphi_2 \rangle + \frac{i}{2} \Omega(\varphi_1, \varphi_2).$$  

The GNS construction for $\omega$ has a natural Fock space structure, i.e.

$$\omega(\hat{A}) = \langle 0|\rho(\hat{A})|0 \rangle \quad \forall \hat{A} \in \mathcal{A}$$  

where

$$\rho(\hat{W}_\varphi) = \exp[a(P^+\varphi) - a^\dagger(\varphi)]$$  

and the Fock vacuum $|0\rangle$ is the cyclic vector of the representation. But in general $\mathcal{H}^+$ is not simply a space of complex solutions, and only $P^+S + iP^+S$ (and not $P^+S$ itself as in the case of a pure state $\omega$) is dense in $\mathcal{H}^+$. The following four statements can be proven to be equivalent (see [2]): (i) $\omega$ is pure, (ii) $\rho$ is irreducible, (iii) $P^+S$ is dense in $\mathcal{H}^+$, (iv) the inner product $\langle \cdot , \cdot \rangle$ obeys the supremum condition (2.26).
3 A “physical” Hilbert space of classical solutions

In this section a certain candidate for an inner product obeying (2.32) or even (2.26) will be constructed. We consider this candidate to be a natural one because it is provided by a certain refinement of the Dirac quantization prescription for constrained systems. This refinement was proposed under the name “refined algebraic quantization” by Ashtekar et al. [1] in the context of the connection dynamics approach to canonical quantum gravity. It is in fact a physicist’s version of what is known as Rieffel induction in pure mathematics [4]. The latter may be considered to be a quantum analog of Marsden–Weinstein reduction (a geometrical construction of a reduced phase space) and of a more general method of constructing new symplectic spaces and Poisson morphisms from old ones [5].

Rather than restating the general principles of the refined algebraic quantization scheme (which can be found in [1]) we shall confine ourselves here to a simplified version that is sufficient for its application to the relativistic particle, and its main points should become clear from the application itself. We start from the reparametrization-invariant action for the relativistic particle in a curved space-time, admitting also a nontrivial “potential” $V$:

$$S[x(\tau)] = -\int [V(x)]^{1/2} ds.$$  (3.1)

This contains the invariant line element

$$ds = \left( g^{ab} \left( \frac{dx^a}{d\tau} \frac{dx^b}{d\tau} \right) \right)^{1/2} d\tau$$  (3.2)

and implies the constraint

$$C \equiv -g^{ab} p_a p_b + V(x) = 0.$$  (3.3)

Quantization according to the refined algebraic scheme proceeds in two steps.

Step 1 consists in the quantization of the “unconstrained” system. In the position representation state vectors are represented by wave functions $\tilde{\psi} \in L^2(M, d^4 x)$ and the canonically conjugate momenta by operators

$$\hat{p}_a : \tilde{\psi} \to i \frac{\partial}{\partial x^a} \tilde{\psi}.$$  (3.4)

Note that it is the requirement that these operators be self-adjoint that distinguishes the non-invariant measure $d^4x$ defining the $L^2$ space. As scalar products have to be invariant, $|\tilde{\psi}|^2$ must be a scalar density. Equivalently, however, we can define scalar wave functions

$$\psi := |g|^{-1/4} \tilde{\psi}$$  (3.5)

which are acted upon by the conjugate momenta as

$$\hat{p}_a : \psi \to |g|^{-1/4} \frac{\partial}{\partial x^a} |g|^{1/4} \psi.$$  (3.6)
These wave functions $\psi$ are elements of an invariantly defined Hilbert space, which has only auxiliary status, however, and will therefore be denoted by $H_{\text{aux}}$:

$$\psi \in H_{\text{aux}} \equiv L^2(M, |g|^{1/2} d^4x).$$

(3.7)

The relevant inner product is given by

$$\langle \varphi, \psi \rangle_{\text{aux}} = \int d^4x \, |g|^{1/2} \varphi \psi.$$  

(3.8)

The quantum version of the constraint requires the factor ordering

$$(g^{ab} \hat{p}_a \hat{p}_b) = |g|^{-1/4} \hat{p}_a |g|^{1/2} g^{ab} |g|^{1/2} g^{bc} \hat{p}_c |g|^{-1/4}$$

(3.9)

so as to yield the local differential operator $\hat{C}$ of (2.5) in the position representation. The operator $\hat{C}$ is unbounded in $H_{\text{aux}}$ and in general the Dirac quantization condition

$$\hat{C} \psi = 0$$

(3.10)

has no solution in $H_{\text{aux}}$.

Step 2 of the refined algebraic quantization scheme defines formally a “physical” Hilbert space of solutions of (3.10). It starts from the subspace

$$D_M \equiv C^\infty_0(M) \subset H_{\text{aux}}$$

(3.11)

which is invariant under $\hat{C}$ provided that $V(x)$ is sufficiently well-behaved. $D_M$ is a nuclear space, the definition of its topology being a straightforward generalization from the case when $M$ is flat (note that there is no such straightforward generalization of Schwartz space to a curved manifold). Since the nuclear topology of $D_M$ is stronger than that induced by the $L^2$ norm, the nuclear dual $D'_M$ is larger than $H_{\text{aux}}$. As the inner product $\langle \cdot, \cdot \rangle_{\text{aux}}$ is continuous with respect to the nuclear topology, there exists an antilinear embedding of $D_M$ in $D'_M$, $\varphi_0 \mapsto \varphi_0'$, defined by

$$\varphi_0'(\psi_0) := \langle \varphi_0, \psi_0 \rangle_{\text{aux}}.$$  

(3.12)

A further antilinear map $\eta : D_M \to D'_M$ called “rigging map”, is defined formally by

$$\eta : \psi_0 \mapsto \psi = 2\pi \delta(\hat{C}) \overline{\psi_0}$$

(3.13)

whence

$$\hat{C} \psi = 0.$$  

(3.14)

A formally positive definite inner product $\langle \cdot, \cdot \rangle_{\text{phys}}$ on $\eta(D_M)$ can be defined by

$$\langle \varphi, \psi \rangle_{\text{phys}} := (\eta \psi_0)(\varphi_0).$$

(3.15)

Finally a Hilbert space $H_{\text{phys}}$ is obtained by completing $\eta(D_M)$ with respect to $\langle \cdot, \cdot \rangle_{\text{phys}}$. This completes the refined algebraic quantization of the relativistic particle. Before discussing its physical significance, we turn to the construction of the formal definitions involved in step 2.
The construction rests on the assumption that the operator $\hat{C}$ is self-adjoint on a dense domain $D \subseteq H_{aux}$ with $D_M \subseteq D$. (Since $\hat{C}$ is a real operator, the existence of self-adjoint extensions is ensured by a theorem of von Neumann.) Thus $\hat{C}$ is continuous on $D_M$ w.r.t. the nuclear topology. As $\hat{C}D_M \subseteq D_M$, one may define the operator $\hat{C}' : D'_M \to D'_M$ by

$$(\hat{C}' f)(\varphi) = f(\hat{C}\varphi). \quad (3.16)$$

The assumption just stated together with the fact that $\langle , \rangle_{aux}$ is continuous on $D_M$ and $D_M$ is dense in $H_{aux}$ allows the application of the nuclear spectral theorem ([8, 9]) with the following result:

There exists a system $\{e_{\lambda k}\}$ of eigenfunctionals of $\hat{C}$ (i.e. $\hat{C}' e_{\lambda k} = \lambda e_{\lambda k}$) such that for any $\varphi_0 \in D_M \varphi'_0$ may be represented as

$$\varphi'_0 = \int_{\sigma} \sum_{k=1}^{m_\lambda} \overline{\varphi_{\lambda k}} e_{\lambda k} d\mu(\lambda) \quad (3.17)$$

where $\sigma$ is the spectrum of $\hat{C}$, $\mu$ is a measure and $m_\lambda$ the multiplicity of the spectral value $\lambda$ (as they are defined in the multiplication operator version of the spectral theorem). Moreover

$$\varphi_{\lambda k} = e_{\lambda k}(\varphi_0). \quad (3.18)$$

From (3.17) we infer the exact definition of the rigging map (3.13):

$$\varphi \equiv \eta \varphi_0 = 2\pi \sum_{k=1}^{m_0} \overline{\varphi_{0k}} e_{0k}. \quad (3.19)$$

Hence the inner product (3.15) is expressed as

$$\langle \varphi, \psi \rangle_{phys} = (\eta \psi_0)(\varphi_0) = 2\pi \sum_{k=1}^{m_0} \overline{\varphi_{0k}} \psi_{0k} \quad (3.20)$$

where we have used (3.18).

If the spectrum of $\hat{C}$ has no singular continuous part, an equivalent definition of $H_{phys}$ is implied by the fact that in the spectral representation the $e_{\lambda k}$ are distributions concentrated in a point $\lambda \in \sigma$. We define the spectral $\delta$ distribution $\delta_{\mu}(\lambda, \lambda')$ by

$$\int_{\sigma} d\mu(\lambda') \delta_{\mu}(\lambda, \lambda') \varphi(\lambda') = \varphi(\lambda) \quad (3.21)$$

for any test function $\varphi$. If $\lambda$ belongs to the pure point spectrum,

$$\delta_{\mu}(\lambda, \lambda') = \delta_{\lambda, \lambda'}. \quad (3.22)$$

If $\lambda$ is in the absolutely continuous (w.r.t. Lebesgue measure) part of the spectrum and hence $d\mu/d\lambda \neq 0$ exists, then

$$\delta_{\mu}(\lambda, \lambda') = \left(\frac{d\mu}{d\lambda}\right)^{-1} \delta(\lambda - \lambda'). \quad (3.23)$$
Note that $\delta(\lambda, \lambda')$ is not translation invariant in general.

The inner product $\langle e_{\lambda k}, e_{\lambda' k'} \rangle_{\text{aux}}$ is defined in the above distributional sense. We may choose the system $\{e_{\lambda k}\}$ to be orthonormal:

$$\langle e_{\lambda k}, e_{\lambda' k'} \rangle_{\text{aux}} = \delta_\mu(\lambda, \lambda')\delta_{k,k'}.$$  \hspace{1cm} (3.24)

It turns out in all known applications (although apparently there is no general proof) that the $e_{\lambda k}$ may be chosen such that they are represented by locally integrable eigenfunctions $e_{\lambda k}(x)$ according to

$$e_{\lambda k}(\varphi) = \int d^4x |g|^{1/2}e_{\lambda k}(x)\varphi(x).$$  \hspace{1cm} (3.25)

Hence the inner product

$$\int d^4x |g|^{1/2}e_{\lambda k}e_{\lambda' k'} = \delta_\mu(\lambda, \lambda')\delta_{k,k'}$$  \hspace{1cm} (3.26)

exists as a spectral distribution. Let now $\varphi^{(\lambda)}$ be a locally integrable solution of $\hat{C}\varphi^{(\lambda)} = \lambda\varphi^{(\lambda)}$. It follows from (3.17), (3.20), (3.25) and (3.26) that

$$\int d^4x |g|^{1/2}\varphi^{(0)}(x)\varphi^{(\lambda)} = 2\pi\delta_\mu(0, \lambda)\langle \varphi^{(0)}, \varphi^{(\lambda)} \rangle_{\text{phys}}.$$  \hspace{1cm} (3.27)

Thus the inner product $\langle \psi, \psi \rangle_{\text{phys}}$ turns out to be the general version of an inner product first proposed by Nachtmann in the special case of the Klein–Gordon equation on de Sitter space \[8\]. The definition (3.27) of the physical inner product is more useful for practical computation although it requires to embed a given solution in a whole family parametrized by $\lambda$ (usually, when $V$ is of the form (2.7) and $m^2 \neq 0$, any exact solution of (2.4) obtained by analytical methods will appear as an analytical function of $\lambda$).

As to the physical significance of $H_{\text{phys}}$, we remark that in general the complexified solution space of Sec. 2, $\mathcal{C} \otimes S$, is a subspace and the charge form $\langle \varphi, \psi \rangle$ is defined on $H_{\text{phys}}$. A notable exception are the exponentially growing solutions (“resonances”) that may exist in a certain type of external electrostatic potential in flat space-time \[10\] and that may lie in the (then complex) space $S$, but not in $H_{\text{phys}}$. A gravitational analog of this situation occurs in de Sitter space \[11\]. This suggests an invariant definition of “exponentially growing” or “complex frequency” solutions $\psi$ of (2.4): They do not belong to $H_{\text{phys}}$, or equivalently, $\int d^4x |g|^{1/2}\bar{\varphi}(x)\psi(x)$ does not exist as a distribution in $\lambda$. The Hilbert space $H_{\text{phys}}$ is somewhat reminiscent of the notion of tempered distributions, but note that $H_{\text{phys}}$ is not a nuclear space and that its closure in $D'_M$ is larger (the closure of the linear span of the system $\{e_{\lambda k}\}$ is larger still, namely identical to $D'_M$ itself).

### 4 Invariantly defined states

The inner product $\langle \psi, \psi \rangle_{\text{phys}}$ constructed in the previous section may be substituted for the inner product $\langle \psi, \psi \rangle$ appearing in the Fock space construction of Sec. 2, and we may investigate the physical meaning of the Fock space defined invariantly in this way. First
we have to check the positivity condition (2.32) for the states so defined. To this end we define an operator $N$ on $H_{\text{phys}}$ by

$$\langle \psi_1, N \psi_2 \rangle_{\text{phys}} = (\psi_1, \psi_2).$$  \hspace{1cm} (4.1)$$

It corresponds to the operator $iJ$ of Sec. 2 and is formally self-adjoint. If (2.32) holds, then

$$\frac{\vert \langle \psi_1, N \psi_2 \rangle_{\text{phys}} \vert}{\| \psi_1 \| \| \psi_2 \|} \leq 1$$  \hspace{1cm} (4.2)$$
and hence

$$\vert N \vert \leq 1.$$  \hspace{1cm} (4.3)$$

This inequality cannot be proven in full generality, but it appears to be a generic property. This will be seen from the integral representation of $N$ that we are going to construct now. As is well known, the $\delta$ distribution appears in the boundary value of a holomorphic function, viz.

$$\frac{1}{x + i0} \equiv \lim_{\varepsilon \downarrow 0} \frac{1}{x + i\varepsilon} = P \frac{1}{x} + i\pi \delta(x)$$  \hspace{1cm} (4.4)$$

($P$ denoting the principal value). Therefore we obtain for the self-adjoint operator $\hat{C}$ the relation

$$2\pi i \delta(\hat{C}) = (\hat{C} - i0)^{-1} - (\hat{C} + i0)^{-1}$$  \hspace{1cm} (4.5)$$

(note that $(\hat{C} \pm i\varepsilon)^{-1}$ is bounded and holomorphic in $\varepsilon$ for $\varepsilon > 0$).

We define the Feynman propagator $K(x, x')$ as the (singular) integral kernel of $(\hat{C} - i0)^{-1}$ with respect to space-time integration:

$$[(\hat{C} - i0)^{-1}\psi](x) = -\int d^4x' |g|^{1/2}K(x, x')\psi(x').$$  \hspace{1cm} (4.6)$$

It is symmetric in its arguments,

$$K(x, x') = K(x', x)$$  \hspace{1cm} (4.7)$$

as is evident from the fact that its complex conjugate $\overline{K}(x, x')$ (called the antipropagator) is the integral kernel of $(\hat{C} + i0)^{-1}$ and therefore equals also its adjoint. Equations (3.13) and (4.5) imply

$$(\eta\psi_0)(x) = \int d^4x' |g|^{1/2}G_1(x, x')\overline{\psi_0}(x')$$  \hspace{1cm} (4.8)$$

where

$$G_1 := i(K - \overline{K})$$  \hspace{1cm} (4.9)$$

is a real symmetric “Green function” (solution of (2.4) in both arguments). Since $G_1$ is the kernel of the identity w.r.t. $\langle \cdot, \cdot \rangle_{\text{phys}},$

$$\psi(x) = \langle G_1(x, \cdot), \psi \rangle_{\text{phys}},$$  \hspace{1cm} (4.10)$$
it is the kernel of $N$ w.r.t. the charge form:

$$\langle N\psi(x), N\psi \rangle_{\text{phys}} = \langle G_1(x, \cdot), \psi \rangle$$

or

$$\langle N\psi(x), N\psi \rangle = i\int d\sigma G_1(x, x') \nabla \cdot \psi(x) \equiv -i(G_1 \ast \psi)(x).$$

For a further evaluation of (4.12) we make use of the chronological decomposition of the Feynman propagator,

$$K(x, y) = \Theta(x, \Sigma(y))G^\uparrow(x, y) - \Theta(\Sigma(y), x)G^\downarrow(x, y),$$

where $\Sigma(y)$ is an arbitrary spacelike Cauchy hypersurface containing $y$, the chronological step function $\Theta(x, \Sigma)$ is one if $x$ is in the chronological future of $\Sigma$ and zero otherwise, and $\Theta(\Sigma, x) = 1 - \Theta(x, \Sigma)$. The kernels $G^\uparrow, G^\downarrow$ solve (2.4) in both arguments. If the domain $D$ of $C$ is characterized by asymptotic fall-off conditions (as is generically the case), then the chronological decompositions of $K$ and $\overline{K}$ define four projection operators:

$$P^\uparrow \psi := G^\uparrow \ast \psi, \quad P^\downarrow \psi := G^\downarrow \ast \psi$$

They obey the relations

$$P = P^\dagger \quad (4.16)$$

$$P^\dagger P^\perp = 0 = \overline{P} \overline{P}^\perp \quad (4.17)$$

$$P^\dagger + P^\perp = \text{id}_{\mathcal{H}_{\text{phys}}} = \overline{P}^\dagger + \overline{P}^\perp \quad (4.18)$$

where the adjoint in (4.16) is defined with respect to $\langle \cdot, \cdot \rangle_{\text{phys}}$. For a derivation of these relations as well as the projection property itself see [9].

From (4.9) and (4.12) – (4.15) we conclude that $N$ is the difference of two projections

$$N = P^\dagger - \overline{P}^\dagger = \overline{P}^\perp - P^\perp,$$

and hence (4.3) and the positivity condition (4.2) do indeed hold. The stronger supremum condition (2.26) is valid exactly if the spectrum of $N$ consists only of $+1$ and $-1$, i.e. if $\overline{P}^\dagger = P^\dagger$ and $P^\perp = \overline{P}^\perp$. In this case the unique Fock space obtained by setting $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{\text{phys}}$ in Sec. 2 is indeed physical, as has been verified in concrete examples [11]. If (2.26) does not hold, a unique irreducible Fock representation may still be defined by choosing $\mathcal{H}^\dagger$ to consist of the eigenfunctions of $N$ corresponding to positive eigenvalues (as was proposed by Nachtmann [8]). This definition does not even require the positivity condition (2.32). However it cannot be correct in general, because strong physical arguments speak against the existence of a unique natural “vacuum” state (e.g. it would preclude the possibility of particle creation by the external field).
In general the physically correct procedure appears to be to use the projection operators (4.14), (4.15) to define two Fock spaces $F^\uparrow_s, F^\downarrow_s$ based on the one-particle Hilbert spaces

$$\mathcal{H}^+ = P^\dagger \mathcal{H}_{\text{phys}}^+, \quad \mathcal{H}_+ = P^\dagger \mathcal{H}_{\text{phys}}^-.$$  \hfill (4.20)

Concrete examples \cite{11} show that $\mathcal{H}_+$ and $\mathcal{H}^+$ define in- and outgoing physical particles, respectively. In particular, particle creation is predicted in this way for space-times where it is expected for physical reasons. The Bogoliubov transformation between the in- and outgoing representation is not unitarily implementable in general, and neither the in- nor the out-vacuum will be Hadamard states (this being a local property in contrast to the global character of our definition of states). Finally, although the mixed quasifree state $\omega$ associated with $\langle \cdot , \cdot \rangle_{\text{phys}}$ via (2.33) is defined in general, it does not seem to have a clear physical interpretation (it will contain contributions of arbitrary particle number in $F^\uparrow_s$ and $F^\downarrow_s$).

5 Concluding remarks: relativistic quantum mechanics

As is well known, perturbative quantum field theory has an equivalent formulation in relativistic quantum mechanics that was developed by Feynman. The main ingredients for the calculation of amplitudes in this approach are the charge form and the Feynman propagator (supplemented by vertex rules in the interacting case). Remarkably, both of these elements are dispensable once the inner product $\langle \cdot , \cdot \rangle_{\text{phys}}$ is introduced. First of all, the one-particle Hilbert spaces may be defined without reference to the Feynman propagator in the following way \cite{9}: Solutions $\psi^{(0)}(0)$ in $\mathcal{H}^+ (\mathcal{H}_+)$ are regular in the asymptotic future (past) upon analytic continuation in the parameter $\lambda$ of the eigenvalue equation $\hat{C}\psi(\lambda) = \lambda \psi(\lambda)$ into the upper (lower) half complex $\lambda$-plane. With this definition of in- and outgoing particle (and antiparticle) states, it can be shown \cite{9} that the inner product $\langle \cdot , \cdot \rangle_{\text{phys}}$ yields directly the physical amplitudes. E.g. the relative amplitude for pair creation in the mode $\psi^*$ is $\langle \psi^*, \psi^* \rangle / \langle \psi^*, \psi^* \rangle$. This version of relativistic quantum mechanics is as self-contained as the nonrelativistic theory (with e.g. pair creation treated as “backscattering into the future”). Yet another approach to relativistic quantum mechanics is the Hamiltonian path-integral quantization of the relativistic particle \cite{12}. It is gratifying to observe that this yields $\langle x | x' \rangle = K(x, x')$ where $K$ is the Feynman propagator as defined in Sec. 4.

In conclusion, then, it appears that refined algebraic quantization does indeed define a physical inner product and Hilbert space of solutions for quantum field theory in curved space-time. The construction has to be supplemented by a proper definition of states, which, however, is suggested by the formalism itself. Moreover it shows that relativistic quantum mechanics is more than just a prelude to quantum field theory.
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