The Free Scalar Quantum Field in Continuous Spacetime

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Abstract This article describes a manifestly Poincaré-symmetric way to construct a simple example of a relativistic quantum field theory.

Contents

1 Motive

Relativistic[1] quantum field theory is the foundation for our current understanding of almost everything we know about nature. Learning relativistic quantum field theory is challenging, because the easiest models are not very realistic and the most realistic models are not very easy. This article introduces a model that is not very realistic, but it is easy, at least compared to most other relativistic models.

In quantum field theory, observables are expressed in terms of field operators. This article introduces a simple model in which the field's time dependence is described by a *linear* equation of motion. This makes the math relatively easy. It also means that the corresponding particles don't interact with each other (article 30983), but the model is still useful as a step toward the study of other models that do include interactions.

One important theme in quantum field theory is that Poincaré symmetry can emerge at sufficiently low resolution even if a model is defined in a way that doesn't have that symmetry exactly,[2] as in **lattice quantum field theory**. Models with exact Poincaré symmetry do exist, but constructing them in a way that makes their Poincaré symmetry manifest is usually not easy. The free scalar model is the easiest example. This article shows how to construct the free scalar model in a way that respects Poincaré symmetry exactly. This is not necessarily the easiest way to construct the free scalar model,[3] but it is at least a relatively easy example of exact Poincaré symmetry in quantum field theory.

[1] The name *relativistic* refers to Poincaré symmetry. A model that has Galilei symmetry instead is called (strictly) *nonrelativistic*. These are just names, not good descriptions, because motion is relative in both cases.

[2] This is a special case of a more general theme called **effective field theory**.

[3] The approach used in article 52890 is arguably easier, and it's also more widely applicable, but it doesn't respect Poincaré symmetry exactly.

2 Preview and notation

Ideally, we would like to associate one or more field operators $\phi(x)$ with each point x of spacetime, using x as an index. Then the set of observables associated with a given region R of spacetime would be contructed from field operators $\phi(x)$ with $x \in R$. However, trying to associate operators with individual points in continuous spacetime causes mathematical trouble. One way to avoid trouble is to discretize spacetime, or at least space, but that's messy and artificial.[4]

For the free scalar field, we have a more pleasant option.[5] Instead of using a point x in spacetime as an index, we can use a smooth function $f(x)$ as an index. The corresponding **field operator** is denoted $\phi(f)$. The association between field operators and regions of spacetime can be expressed in terms of the index functions, and so can the commutation relations. The whole construction respects Poincaré symmetry exactly. Sections 15-16 will explain how this approach relates to the more traditional approach that tries to use a point in spacetime as an index.

In this article, spacetime is flat (article 48968). The spacetime coordinates are denoted x^a with $a \in \{0, 1, 2, ..., D\}$. The standard abbreviations $\partial_a \equiv \partial/\partial x^a$ and $\partial^a \equiv \eta^{ab}\partial_b$ are used, with an implied sum[6] over b, where η^{ab} are the components of the inverse metric tensor:

$$\eta^{ab} = \begin{cases} 1 & \text{if } a = b = 0, \\ -1 & \text{if } a = b > 0, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

An alternative notation that treats the time coordinate $t \equiv x^0$ differently than the others will be used for some things, starting in section 8.

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[4] It's messy and artificial, but it's also even easier – both conceptually and mathematically – than the approach used in this article, and it works for a much larger variety of models. Article 52890 shows how to construct a discrete-space version of a family of models that includes the free scalar model as a special case.

[5] The approach used here only works in models whose equations of motion are linear. More information about this approach is given in section 2.1 in Hollands and Wald (2014) and the references it cites.

[6] A sum is implied over any spacetime index that is repeated in the same term.

3 The field operators

We could start with a Hilbert space and then describe the field operators as things that act on the Hilbert space. This article does the opposite: it starts with the field operators and then gives them a Hilbert space to act on (section 13).

A **field operator** will be denoted $\phi(f)$, where the function f is used an index. Let $\mathcal{F}$ denote the set of allowed "values" of this index. The set $\mathcal{F}$ will be specified in sections 4 and 6. For each $f \in \mathcal{F}$, we have a field operator $\phi(f)$. The map from index functions to field operators is linear, which means

$$\phi(z_1 f_1 + z_2 f_2) = z_1 \phi(f_1) + z_2 \phi(f_2) \tag{2}$$

for all functions $f_1, f_2 \in \mathcal{F}$ and all complex numbers z_1, z_2. In particular, if $f = 0$, then $\phi(f) = 0$. The adjoint of $\phi(f)$ will be denoted $\phi^*(f)$ and is given by

$$\phi^*(f) = \phi(f^*) \tag{3}$$

where f^* denotes the complex conjugate of the function f. The commutation relations for the free scalar model are

$$\big[\phi(f), \phi^*(g)\big] = (f, g), \tag{4}$$

where (f, g) is a complex number that will be defined in section 5.[7,8]

[7]The right-hand side of (4) is an abbreviation for the complex number (f, g) times the identity operator.

[8]The fact that the right-hand side of equation (4) is proportional to the identity operator implies the field operators must be *unbounded* (theorem III.2 in Speicher (2020)), which means that they are defined only on a dense subset of the Hilbert space instead of on the whole Hilbert space.

4 The index functions, part 1

Section 3 referred to a set $\mathcal{F}$ of index functions. As a step toward defining the set $\mathcal{F}$, this section defines two related sets: a larger set $\mathcal{F}_1$ that contains $\mathcal{F}$, and a smaller set $\mathcal{F}_0$ that is contained within $\mathcal{F}$. In symbols:

$$\mathcal{F}_0 \subset \mathcal{F} \subset \mathcal{F}_1. \tag{5}$$

To define the larger set $\mathcal{F}_1$, choose a positive real number $m > 0$.[9] The larger set $\mathcal{F}_1$ is the set of all smooth complex-valued functions f that satisfy the **Klein-Gordon equation**

$$\partial^a \partial_a f(x) + m^2 f(x) = 0, \tag{6}$$

using the notation that was defined in section 2.

To define the smaller set $\mathcal{F}_0$, let Σ be a spacelike hypersurface,[10] and let n be a future-pointing unit vector field that is orthogonal[11] to Σ everywhere on Σ. For any complex-valued function f, its **initial data** consists of its values at all points of Σ together with its normal derivative $n^a \partial_a f$ at all points of Σ. The smaller set $\mathcal{F}_0$ consists of functions $f \in \mathcal{F}_1$ whose initial data have compact support on Σ.[12]

Article 98038 shows that equation (6) has the **causality property**, so if f is a solution whose initial data have compact support on Σ, then its initial data have compact support on *every* spacelike hypersurface Σ. As a result, $\mathcal{F}_0$ may also be described as the set of solutions of (6) whose initial data have compact support on every spacelike hypersurface Σ.

This section defined the sets $\mathcal{F}_0$ and $\mathcal{F}_1$ in (5). The middle set $\mathcal{F}$ in (5) – the set of index functions – will be defined in section 6.

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[9] This will turn out to be the mass of a single particle (article 30983).

[10] A **hypersurface** is a submanifold with one less dimension than the ambient manifold (Berger (2003), section 4.1.3.1). Space at time $t = 0$ is a hypersurface in spacetime.

[11] *Orthogonal* is defined by the Minkowski metric (1). The normal vector n must be timelike, because Σ is spacelike.

[12] This means that f and $n^a \partial_a f$ are both zero everywhere on Σ except within a bounded subset of Σ.

5 The invariant product of index functions, part 1

The quantity (f, g) on the right-hand side of equation (4) will be defined in section 9 for all index functions. This section defines it for index functions in the smaller set $\mathcal{F}_0$. These functions are solutions of (6) whose initial data have compact support on every spacelike hypersurface Σ.

For any two complex-valued functions f, g, define

$$j_a(f, g) \equiv i\big(f^* \partial_a g - g \partial_a f^*\big) \tag{7}$$

where i is the imaginary unit ($i^2 = -1$). Both sides of (7) are functions of the spacetime coordinates x, so equation (7) is an abbreviation for

$$j_a(f, g)(x) \equiv i\big(f^*(x) \partial_a g(x) - g(x) \partial_a f^*(x)\big).$$

As in section 4, let Σ be a spacelike hypersurface, and let n be a future-pointing unit vector field that is orthogonal to Σ everywhere on Σ. If either f or g is in $\mathcal{F}_0$, then $j_a(f, g)$ has compact support on Σ, so the integral

$$(f, g)_\Sigma \equiv \int_\Sigma n^a j_a(f, g) \tag{8}$$

is finite. If f and g are both in $\mathcal{F}_1$, then equation (6) implies

$$\partial^a j_a(f, g) = 0. \tag{9}$$

Now supppose that f and g are both in the larger set $\mathcal{F}_1$ and that at least one of them is also in the smaller set $\mathcal{F}_0$. In this case, we can use (9) to prove that the quantity (8) is the same for all spacelike hypersurfaces Σ. To do this, let $\mathcal{M}$ be any region of spacetime bounded by two spacelike hypersurfaces Σ_1 and Σ_2. Equation (9) implies

$$\int_\mathcal{M} \partial^a j_a(f, g) = 0,$$

and since $j_a(f,g)$ has compact support within $\mathcal{M}$, we can use integration-by-parts to get

$$\int_{\partial\mathcal{M}} n^a j_a(f,g) = 0, \tag{10}$$

where $\partial\mathcal{M}$ denotes the (oriented) boundary of $\mathcal{M}$. This boundary consists of Σ_1 and Σ_2, oriented so that their contributions to the integral have the opposite sign, so equation (10) may also be written

$$\int_{\Sigma_1} n^a j_a(f,g) - \int_{\Sigma_2} n^a j_a(f,g) = 0. \tag{11}$$

This says that the quantity (8) is the same no matter which spacelike hypersurface we use, so we can write it as

$$(f,g) \tag{12}$$

without the subscript Σ, at least if f, g satisfy the assumed conditions.

The quantity (12) will be called the **invariant product**, because it's invariant under Poincaré transforms (section 12). Poincaré symmetry and the Σ-independence property (11) are both preserved when the definition of (f,g) is extended to all index functions in $\mathcal{F}$, which will be done in section 9. That extension is the quantity on the right-hand side of (4).

6 The index functions, part 2

This section defines the set $\mathcal{F}$ of index functions, as promised in section 4.

A function in $\mathcal{F}_0$ can be written like this:

$$f(x) = \int \frac{d^{1+D}k}{(2\pi)^{1+D}}\, 2\pi\delta(k_a k^a - m^2)\, \exp\big(-ik_a x^a\big)\, \tilde{f}(k), \tag{13}$$

for some complex-valued $\tilde{f}(k)$, where $\delta(\cdots)$ is the Dirac delta distribution[13] defined by the relationship

$$\int_{-\infty}^{\infty} du\; g(u)\delta(u) = g(0) \tag{14}$$

for all sufficiently well-behaved functions $g(u)$ of a single real variable u. The integral (13) may be written as a sum of two terms, one involving only $k_0 > 0$ and one involving only $k_0 < 0$. These two terms will be called the **positive-** and **negative-frequency** parts of $f(x)$, respectively. Let K and $\overline{K} \equiv 1 - K$ be the projections onto these two parts, so

$$f = Kf + \overline{K}f \tag{15}$$

$$K^2 = K. \tag{16}$$

Now we can finally define $\mathcal{F}$: it is the set of all linear combinations of functions from $K\mathcal{F}_0$ and $\overline{K}\mathcal{F}_0$.

The set $\mathcal{F}$ is larger than $\mathcal{F}_0$. Even if f has compact support on every spacelike hypersurface, Kf might not have compact support on *any* spacelike hypersurface. Section 9 will explain how the definition of the invariant product introduced in section 5 can be extended to the larger set $\mathcal{F}$.

[13] It is occasionally called a "function," but it is technically a **tempered distribution** (article 58590), not a function.

7 Some properties of the projection

- The decomposition into positive- and negative-frequency parts is not affected by Poincaré transforms, because it depends only on the sign (not the value) of the timelike component of k. This shows that the set $\mathcal{F}$ is self-contained under Poincaré transforms.

- Equation (13) says that taking the complex conjugate of $f(x)$ is the same as replacing $\tilde{f}(k) \to \tilde{f}^*(-k)$ in the integrand, so the projection K satisfies

$$(Kf)^* = \overline{K} f^*. \tag{17}$$

  Equations (15) and (17) imply

$$Kf + (Kf)^* = Kf + \overline{K} f = f \qquad \text{if } f^* = f.$$

  This shows that if $f \in \mathcal{F}_0$ is real, then f is uniquely determined by Kf.

8 A more explicit formulation

Using a notation that separates the time and space components makes Poincaré symmetry less obvious, but it can also have advantages. Use the notation $x = (t, \mathbf{x})$ and $k = (k_0, \mathbf{k})$ and

$$\omega(\mathbf{k}) \equiv \sqrt{\mathbf{k}^2 + m^2} \tag{18}$$

and the identity[14]

$$\delta(k_a k^a - m^2) = \frac{\delta\big(k_0 - \omega(\mathbf{k})\big) + \delta\big(k_0 + \omega(\mathbf{k})\big)}{2\omega(\mathbf{k})} \tag{19}$$

to write the positive- and negative-frequency parts as

$$\begin{aligned} Kf(t,\mathbf{x}) &\equiv \int \frac{d^D k}{(2\pi)^D\, 2\omega}\ \exp\big(-i\omega t\big)\ \exp\big(-i\mathbf{k}\cdot\mathbf{x}\big)\ \tilde{f}(\omega,\mathbf{k}) \\ \overline{K}f(t,\mathbf{x}) &\equiv \int \frac{d^D k}{(2\pi)^D\, 2\omega}\ \exp\big(i\omega t\big)\ \exp\big(-i\mathbf{k}\cdot\mathbf{x}\big)\ \tilde{f}(-\omega,\mathbf{k}) \\ &= \int \frac{d^D k}{(2\pi)^D\, 2\omega}\ \exp\big(i\omega t\big)\ \exp\big(i\mathbf{k}\cdot\mathbf{x}\big)\ \tilde{f}(-\omega,-\mathbf{k}). \end{aligned} \tag{20}$$

[14]Here's an outline of a proof of (19). One of the criteria for a function $g(u)$ in (14) to be "sufficiently well-behaved" is that it allows using integration-by-parts with no contributions from $u = \pm\infty$. For such functions,

$$-\int_0^\infty du\ \frac{d}{du}g(u) - \int_{-\infty}^\infty du\ \theta(u)\frac{d}{du}g(u) = g(0),$$

where $\theta(u)$ equals 1 for $u > 0$ and equals 0 for $u < 0$. Compare this to (14) to get $\delta(u) = \frac{d}{du}\theta(u)$, with the understanding that both sides belong inside an integrand with a sufficiently well-behaved function. Now apply d/dx to the straightforward identity

$$\theta(x^2 - \omega^2) = \theta(x - \omega) + 1 - \theta(x + \omega)$$

to get

$$2x\,\delta(x^2 - \omega^2) = \delta(x - \omega) - \delta(x + \omega).$$

Divide both sides by $2x$ and then use the δs on the right-hand side to replace x with $\pm\omega$. This gives (19).

9 The invariant product of index functions, part 2

Section 5 defined the invariant product (f, g) when the functions f and g are both in the larger set $\mathcal{F}_1$ and at least one of them is in the smaller set $\mathcal{F}_0$. This section extends the definition of (f, g) to all index functions $f, g \in \mathcal{F}$. This will be used in section 13 to construct a Hilbert space for the field operators to act on.

The projection K that was defined in section 6 satisfies[15]

$$(Kf, g) = (f, Kg) \tag{21}$$

for all pairs $f, g \in \mathcal{F}$ for which (f, g) was defined in section 5. This says that (f, Kg) is independent of $\overline{K}f$, so we can define

$$(Kf, Kg) \equiv (f, Kg). \tag{22}$$

This extends the definition of the invariant product to all $f, g \in \mathcal{F}$. Equations (21)-(22) may be used together with (16) to deduce

$$(Kf, \overline{K}g) = 0. \tag{23}$$

These equations may also be used to show that the Σ-independence property that was derived in section 5 holds for all $f, g \in \mathcal{F}$.

[15]To derive this, start with the definition (7) of $j_a(f, g)$ and write f and g as in (13). Doing the integral over x reduces the two k-integrals (with different ks) to a single k-integral (with the same k). The δ in (13) implies that k is timelike. If either of the functions f and g is restricted to positive frequencies, then the resulting single k-integral inherits this restriction. The resulting k-integral is the same whether the restriction was inherited from f or g, and equation (21) is just another way of expressing this statement.

10 The sign of the invariant product

This section derives the result

$$(Kf, Kf) > 0 \qquad \text{if } Kf \neq 0, \tag{24}$$

which can then be used to deduce[16]

$$(\overline{K}f, \overline{K}f) \leq 0 \tag{25}$$

$$(\overline{K}f, \overline{K}f) = -(Kf, Kf) \qquad \text{if } f \text{ is real.} \tag{26}$$

To derive (24), remember that the quantity (8) is independent of Σ, so we might as well choose Σ to be a hypersurface of constant x^0. This gives

$$\begin{aligned}(f, g) &= \int d^D x \; j_0(f, g) \\ &= i \int d^D x \; \left(f^* \dot{g} - g \dot{f}^*\right)\end{aligned} \tag{27}$$

where the integral is only over the "spatial" coordinates of x, and an overhead dot denotes a derivative with respect to the "time" coordinate $t \equiv x^0$. Use the definition (22) together with equations (20) and (27) to get

$$(Kf, Kf) \equiv (f, Kf) = \int \frac{d^D k}{(2\pi)^D} \; \left|\tilde{f}(\omega, \mathbf{k})\right|^2,$$

which is positive if $\tilde{f}(\omega, \mathbf{k}) \neq 0$. This implies (24).

[16] To deduce (25), use equation (7) to get $(f, g)^* = -(f^*, g^*)$, then use (17) and (24). To deduce (26), use equation (7) to see that $(f, f) = 0$ when f is real, and then use $f = Kf + \overline{K}f$ and (23).

11 Observables

To specify a model, we need to specify its observables. First, here are some definitions:

- A **causal** worldline is a worldline that is not spacelike anywhere (article 48968).
- For any region R of spacetime, its **causal complement** R' consists of all points in spacetime that cannot be connected to any point in R by any causal worldline.
- Let $\mathcal{F}(R)$ consist of all functions in $\mathcal{F}$ such that $f(x) = 0$ for all $x \in R'$. Article 98038 relates this to the causality property of equation (6).
- Let $\Omega(R)$ be the algebra generated by the field operators $\phi(f)$ with $f \in \mathcal{F}(R)$.

Here is the key principle:

> For any region R of spacetime, observables localized in R are represented by operators in $\Omega(R)$.

In particular, if $\phi(f)$ is self-adjoint and $f \in \mathcal{F}(R)$, then the field operator $\phi(f)$ itself represents an observable localized in R.

We can take R to be an arbitrarily small open[17] neighborhood of a point. We can't take R to be a single point, because then the only smooth function in $\mathcal{F}(R)$ would be $f = 0$, but section 15 describes a devious way to formalize the idea of an observable at a point. Article 52890 describes a more straightforward way.

[17] *Open* is defined by the topological structure (article 93875).

12 Some properties of the model

We haven't yet constructed a Hilbert space for the field operators to act on (that will be done in section 13), but the model constructed in the preceding sections already satisfies these general principles of relativistic quantum field theory:

- **Poincaré symmetry.** If $f \in \mathcal{F}$ and if $x \to \Lambda x$ is a Poincaré transform, then the function f^Λ defined by $f^\Lambda(x) \equiv f(\Lambda x)$ is also in $\mathcal{F}$. More concisely: $\mathcal{F}$ is self-contained under Poincaré transforms. Combine this with (11) to deduce that $(f^\Lambda, g^\Lambda) = (f, g)$ for every Poincaré transform Λ. In other words, the quantity (f, g) on the right-hand side of the commutation relation (4) is invariant under Poincaré transforms.

- **The time-slice principle** (article 22871). Suppose that every causal world-line through R also goes through R_1. Then $R'_1 \subset R'$, which implies $\Omega(R) \subset \Omega(R_1)$ (because if $f(x) = 0$ for all $x \in R'$, then $f(x) = 0$ for all $x \in R'_1 \subset R'$). This is the local version of the time-slice principle (article 21916).

- **Microcausality** (article 21916). This is clear from the fact that $(f, g) = 0$ whenever a spacelike hypersurface Σ exists on which the supports of f and g do not overlap.

Section 13 constructs representation of the algebra of field operators on a Hilbert space, and section 14 shows that it satisfies the **spectrum condition** (article 21916).

13 The Hilbert space

The same algebra of field operators has various Hilbert-space representations that are not all unitarily equivalent to each other. This section constructs a special representation in which the spectrum of the generator of time translations has a finite lower bound. This is called the **vacuum representation**.

To construct the Hilbert space, start with a state $|0\rangle$ defined by these two conditions:[18]

$$\langle 0|0\rangle = 1 \qquad\qquad \phi(Kf)|0\rangle = 0 \qquad \text{for all } f \in \mathcal{F}. \tag{28}$$

The rest of the Hilbert space is generated by applying field operators to this one state-vector. The inner product between any two state-vectors can be worked out using the algebra of field operators (equation (4)), because the Hilbert space is spanned by states of the form

$$\phi^*(f_1)\phi^*(f_2)\cdots\phi^*(f_N)|0\rangle \qquad\qquad \text{with } f_j \in K\mathcal{F}, \tag{29}$$

with any number $N \in \{0, 1, 2, ...\}$ of factors in the product. As an example, consider the state-vectors $|a\rangle \equiv \phi^*(Kf)|0\rangle$ and $|b\rangle \equiv \phi^*(Kg)|0\rangle$. Use equations (4) and (28) to get

$$\langle a|b\rangle = \langle 0|\phi(Kf)\phi^*(Kg)|0\rangle = \langle 0|\big[\phi(Kf), \phi^*(Kg)\big]|0\rangle = (Kf, Kg).$$

Thanks to the inequality (24), this is positive when $f = g$.

To qualify as a Hilbert space, the inner product of *every* state-vector with itself must be positive, and the general principles of quantum theory also require the Hilbert space to be separable. To confirm that these conditions are both satisfied, start with the fact that we can choose a countable sequence of positive-frequency functions $g_1, g_2, ... \in K\mathcal{F}$ whose linear combinations are dense[19] in $K\mathcal{F}$. One

[18] K is the projection defined in section 6.

[19] In other words, any function in $K\mathcal{F}$ can be arbitrarily well-approximated by linear combinations of the g_js.

example of such a sequence is

$$g_j(t,\mathbf{x}) \propto \int \frac{d^D k}{(2\pi)^D}\ \exp\big(-i\omega t\big)\,\omega^{-1/2}\tilde{g}_j(\mathbf{k})\,\exp\big(-i\mathbf{k}\cdot\mathbf{x}\big)$$

where each $\tilde{g}_j(\mathbf{k})$ is $\exp(-\mathbf{k}^2/2)$ times a product of powers of the components of $\mathbf{k}$. These functions are not mutually orthogonal with respect to the invariant product $(\cdot,\cdot)$, but we can use the **Gram-Schmidt process** to derive a sequence of mutually orthogonal functions f_j whose linear combinations are dense in $K\mathcal{F}$. State-vectors of the form (29) still span the Hilbert space when the functions f_j are restricted to this set, and now equations (4) and (28) imply that the inner product of any two such states is a product of factors of the form (f_j, f_k), which is positive if $j = k$ and is zero otherwise. As a result, any two such states are either proportional to each other or orthogonal to each other, and the inner product of any one of them with itself is positive. Every state-vector is (arbitrarily well-approximated by) a linear combination of these, so this implies that the inner product of any state-vector with itself is positive, as required. The fact that the sequence of orthogonal functions f_j is countable also implies that the Hilbert space is separable, as required.

14 The spectrum condition

This section sketches a proof that the model constructed in the previous sections satisfies the spectrum condition. The spectrum condition says that the hamiltonian H, the operator that generates translations in time, should be such that $\langle\psi|H|\psi\rangle$ has a finite lower bound among all unit state-vectors $|\psi\rangle$. The construction in the preceding sections didn't refer to a hamiltonian, but it's implicit in the relationship

$$\langle\psi|H|\psi\rangle = \langle\psi|i\frac{d}{dt}|\psi\rangle, \tag{30}$$

which holds for all time-dependent state-vectors in the Schrödinger picture.

Translating a state of the form (29) forward in time by an amount t' is the same as inserting a factor of $\exp(-i\omega t')$ into the integrand of (20) for each of the functions f_j in (29), so for those states, the right-hand side of (30) involves factors of the form $(f_j, \dot{f}_k)$.[20] To handle this, partition $\mathbf{k}$-space into nonoverlapping cells C and suppose that the functions f_j in (29) all have the form[21]

$$f_j(t,\mathbf{x}) = \int_{\mathbf{k}\in C_j} \frac{d^D k}{(2\pi)^D}\,\frac{\exp(-i\omega t - i\mathbf{k}\cdot\mathbf{x})}{\sqrt{2\omega}},$$

where each C_j is a cell in the partition. The key property of these functions is that if the cells that define f_j and f_k don't overlap, then (f_j, f_k) and $(f_j, \dot{f}_k)$ are *both* zero. Combine this with $\omega > 0$ to deduce that the right-hand side of (30) is positive for all linear combinations of such states. By making the sizes of the $\mathbf{k}$-space cells arbitrarily small, any state can be approximated arbitrarily well by such a linear combination, so this implies that the spectrum condition is satisfied.

[20] In this sentence, the functions f_j can be any index functions, not necessarily the special set of index functions constructed at the end of section 13.

[21] Because of the simplistic way $\mathcal{F}$ was defined in this article, these functions might not belong to $\mathcal{F}$, but they are effectively incorporated when the inner product space constructed in section 13 is completed (in the sense described in article 90771) to obtain a Hilbert space.

15 Field operators at a point

The construction described in the preceding sections is manifestly Poincaré symmetric, but it also has a disadvantage: it only works for free fields (no interactions!). Most traditional introductions to quantum field theory use a different approach, one that associates a pseudo-operator $\phi(x)$ with each individual point x in spacetime. This section, together with section 16, explains how the two approaches are related to each other.

I'm calling $\phi(x)$ a **pseudo-operator** because it is not well-defined as an operator on the Hilbert space, not even on a dense subset of the Hilbert space,[22] but we can manipulate it in some ways as though it were. Most quantum field theory textbooks just call it an operator, which is fine as long as we remember that it really isn't.

The pseudo-operators $\phi(x) = \phi(t, \mathbf{x})$ are self-adjoint, the equation of motion that defines their time-dependence is

$$\partial^a \partial_a \phi(x) + m^2 \phi(x) = 0, \tag{31}$$

and they satisfy the equal-time commutation relations

$$[\phi(t, \mathbf{x}), \phi(t, \mathbf{y})] = 0 \qquad\qquad [\phi(t, \mathbf{x}), \dot{\phi}(t, \mathbf{y})] = i\delta^D(\mathbf{x} - \mathbf{y}), \tag{32}$$

where $\dot{\phi}$ is the derivative of ϕ with respect to t. The $\delta^D(\mathbf{x} - \mathbf{y})$ on the right-hand side is not a function (it doesn't have a value at $\mathbf{x} = \mathbf{y}$), so $\phi(t, \mathbf{x})$ cannot be a well-defined operator on the Hilbert space. To see why these formal rules can still be useful, suppose $f \in \mathcal{F}_0$ and write the field operator $\phi(f)$ as[23]

$$\phi(f) = -i(f, \phi) \equiv \int d^D x \, \big(f^*(t, \mathbf{x}) \dot{\phi}(t, \mathbf{x}) - \phi(t, \mathbf{x}) \dot{f}^*(t, \mathbf{x}) \big). \tag{33}$$

[22] We can make it a legitimate operator on (a dense subset of) the Hilbert space by treating space as a lattice, as in articles 52890 and 00980. That approach ruins exact Poincaré symmetry, but it can be used for a large variety of models.

[23] This corresponds to equation (10) in Hollands and Wald (2014), which uses the term **symplectically smeared** for this way of expressing $\phi(f)$ in terms of $\phi(t, \mathbf{x})$. The factor of i is needed so that $\phi(f)$ is self-adjoint when f is real-valued. Despite appearances, the right-hand side is actually independent of t. This fact is derived below.

Then equations (32) and (33) can be used to reproduce the commutation relation (4). They also imply

$$\big[\phi(t,\mathbf{x}),\, \phi^*(f)\big] = i\, f(t,\mathbf{x}), \tag{34}$$

which is zero when $\mathbf{x}$ is outside the support of f at time t, so the interpretation of $\phi(f)$ established in section 11 is consistent with interpreting $\phi(t,\mathbf{x})$ as being localized at $\mathbf{x}$ at time t.

On the right-hand side of (33), the integrand is a function of t, but the integral is independent of time. To confirm this, take the time-derivative and use equations (6) and (31) to get

$$\frac{d}{dt}\phi(f) = \int d^D x\, \big(f^*(t,\mathbf{x})\nabla^2\phi(t,\mathbf{x}) - \phi(t,\mathbf{x})\nabla^2 f^*(t,\mathbf{x})\big) \tag{35}$$

and then use integration-by-parts to confirm that the integral is zero.

16 Using plane waves as index functions

Sections 4-6 defined the set $\mathcal{F}$ of index functions so that the invariant product (f, g) is a finite complex number for all $f, g \in \mathcal{F}$. If we relax that requirement, then we can relate the approach used in this article to the plane-wave formalism used in many introductions to quantum field theory. Specialize equation (33) to

$$a(\mathbf{k}) \equiv \phi(p_\mathbf{k}) \qquad \text{with } p_\mathbf{k}(t, \mathbf{x}) \equiv \frac{\exp\big(-i\omega(\mathbf{k})t + i\mathbf{k}\cdot\mathbf{x}\big)}{i\sqrt{2\omega(\mathbf{k})}}. \tag{36}$$

The previous section showed that these operators are actually independent of t. Formally, equation (27) gives

$$(p_\mathbf{k}, p_{\mathbf{k}'}) = (2\pi)^D \delta^D(\mathbf{k}' - \mathbf{k}).$$

Use this in the commutation relation (4) to get[24]

$$\big[a(\mathbf{k}),\, a(\mathbf{k}')\big] = 0 \qquad\qquad \big[a(\mathbf{k}),\, a^*(\mathbf{k}')\big] = (2\pi)^D \delta^D(\mathbf{k}' - \mathbf{k}). \tag{37}$$

Use this to confirm that the equation of motion (31) and the commutation relations (32) are both satisfied by

$$\phi(t, \mathbf{x}) = \int \frac{d^D k}{(2\pi)^D} \, \frac{e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}) + \text{adjoint}}{\sqrt{2\omega}}. \tag{38}$$

Substituting this into the right-hand side of (33) with $f = p_\mathbf{k}$ reproduces the definition (36). The construction of the Hilbert space described in section 13 can be expressed in terms of the pseudo-operators $a(\mathbf{k})$ by using the fact that any positive-frequency index function $f \in K\mathcal{F}$ may be expressed in the form

$$f(t, \mathbf{x}) = \int \frac{d^D k}{(2\pi)^D} \, \tilde{f}(\mathbf{k}) p_\mathbf{k}(t, \mathbf{x})$$

for some $\tilde{f}(\mathbf{k})$, with $p_\mathbf{k}$ defined by (36).

[24] I'm writing $a^*(\mathbf{k})$ for the adjoint of $a(\mathbf{k})$. This notation is common in the mathematical literature.

17 A generalization

The plane-wave formalism shown in the previous section can be generalized. Let $\mathcal{M} \subset K\mathcal{F}_1$ be a collection of positive-frequency solutions of equation (6),[25] and write

$$\phi(x) = \sum_{g\in\mathcal{M}} \big(i\phi(g)g(x) + \text{adjoint}\big). \tag{39}$$

If we take $\mathcal{M}$ to be the set of positive-frequency plane-wave functions $p_{\mathbf{k}}$, then (39) reduces to (38).[26] The ansatz (39) is manifestly self-adjoint, and it automatically satisfies the equation of motion (31) because $\mathcal{M} \subset \mathcal{F}_1$ (section 4). Requiring consistency with (34) gives the condition

$$\sum_{g\in\mathcal{M}} (f,g)g^*(x) - \sum_{g\in\mathcal{M}} (f,g^*)g(x) = f^*(x).$$

If $f \in \mathcal{M}$, then equations (17) and (23) say that this reduces to[27]

$$\sum_{g\in\mathcal{M}} (g,f)g(x) = f(x) \qquad\qquad \text{if } f \in \mathcal{M}. \tag{40}$$

Requiring consistency with (32) gives[28]

$$\sum_{g\in\mathcal{M}} \big(g(t,\mathbf{x})g^*(t,\mathbf{y}) - \text{cc}\big) = 0 \tag{41}$$

$$\sum_{g\in\mathcal{M}} \big(g(t,\mathbf{x})\dot{g}^*(t,\mathbf{y}) - \text{cc}\big) = i\delta^D(\mathbf{x}-\mathbf{y}), \tag{42}$$

where "cc" means the complex conjugate of the preceding term. The choice of $\mathcal{M}$ used in section 16 satisfies conditions (40)-(42).

[25] Mnemonic: $\mathcal{M}$ stands for **modes**.

[26] In this case, the formal sum over $g \in \mathcal{M}$ is an integral over $\mathbf{k}$.

[27] To deduce this, use $(f,g)^* = (g,f)$.

[28] To deduce this, use equations (4), (27), and (40).

18 References

(Open-access items include links.)

Berger, 2003. *A Panoramic View of Riemannian Geometry.* Springer

Hollands and Wald, 2014. "Quantum fields in curved spacetime" https://arxiv.org/abs/1401.2026

Speicher, 2020. "Mathematical Aspects of Quantum Mechanics" https://www.uni-saarland.de/fileadmin/upload/lehrstuhl/speicher/Math_of_QM/MathematicalAspects.pdf

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