The Free Scalar Quantum Field: Particles

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Abstract Quantum field theory (QFT) is the foundation for our current understanding of particle physics. One important thing to understand about QFT is how the phenomena we call *particles* arise naturally from a model that is defined entirely in terms of quantum fields, and a first step toward that understanding is to formulate the concept of *particle* using only observables that are available in QFT. This can be done by using observables that act like detectors. This article uses the relativistic free scalar model as an example.

One key message is that in relativistic QFT, perfectly reliable detectors cannot be perfectly localized in any finite region of space. This might not matter much in practical applications, which are never perfect anyway, but it is fundamental to a good understanding of relativistic QFT.

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1 Introduction

In a typical high-energy particle physics experiment, the number of particles can change: the number that comes out may differ from the number that went in. In the context of quantum theory, this implies that the number of particles can be ill-defined: if $|a\rangle$ and $|b\rangle$ are state-vectors with different numbers of particles, then $|a\rangle + |b\rangle$ is a state-vector that doesn't have a well-defined number of particles. Such superpositions must be allowed if the theory includes observables O for which $\langle a|O|b\rangle \neq 0$, as it must if the number of particles can change.

If the number of particles can be ill-defined, then observables can't be tied to particles. In quantum field theory (QFT), observables are tied to spacetime instead, because spacetime doesn't change in QFT.[1] In this framework, the concept of *particle* can be defined in terms of observables that act like particle detectors. The number and arrangement of detectors can be still be well-defined even if the number and arrangement of particles is not. In this way, QFT predicts the very *existence* of particles: when a model is defined in a way that doesn't rely on perturbation theory, the existence of particles is something we get out of the model, not something we arbitrarily put into it.[2]

This article uses the free scalar model to illustrate the idea of using observables that act like detectors to define the particle concept itself. The free scalar model doesn't have any interactions between particles, but the number of particles can still be ill-defined: the model's local observables necessarily mix states with different numbers of particles, even though the hamiltonian (the generator of time translations) does not.

[1] This is a problem for (nonperturbatively) reconciling general relativity with quantum field theory, because the geometry of spacetime is not fixed in general relativity. The AdS/CFT correspondence gets around this problem by tying observables to the asymptotic structure (the "boundary") of spacetime instead of to the bulk of spacetime. The asymptotic geometry is fixed even though the bulk geometry is not. Some references are cited in article 21916.

[2] A model's predictions depend on its input parameters, so of course we can modify a model's particle content by modifying its inputs. We can use this to design a model with a desired particle content, like Weinberg (1995) does in the context of perturbation theory. Even in that context, the particle content is constrained in interesting ways (Weinberg (1996), section 22.4).

2 Using detectors to define the particle concept

To define *particle* in QFT, we should express the definition using observables that are available in QFT. We can do this by using observables that act like detectors. We shouldn't expect to find any definition of *particle* in QFT that perfectly matches the way the word is typically used, because typical usages of the word are influenced by a mental image of the world that isn't consistent with QFT. The real goal here is not to propose any final definition of the word, but rather to learn something about QFT by thinking about how to recognize particle-like phenomena using the observables that QFT provides. Characteristics of particle-like phenomena include:

- Particles can be localized in space.[3]
- Particles can be counted, at least when they're far enough away from each other to avoid confusion.
- A state with one or more particles has higher energy than a state with none.

Here's a first attempt to express those characteristics in terms of detectors:

- Ideally, a detector should be represented by an observable localized in a small region of space.
- Ideally, if a state can can simultaneously trigger up to N well-separated detectors (separated so that they don't disrupt each other), but not more than N well-separated detectors (not even after waiting for **dispersion** as defined in article 20554), then it should qualify as an N-particle state.
- Ideally, the lowest-energy state shouldn't trigger any detector.

All of these conditions start with the word *ideally* because they are not strictly compatible with each other in relativistic QFT, not even in simple toy models like the free scalar model. They are close enough to being consistent with each other

[3]The words "can be" are in this sentence because any superposition of one-particle states should still qualify as a one-particle state, even if the superposition makes the particle nonlocalized.

for practical applications, but uncovering why they're not *strictly* compatible with each other will teach us something important about relativistic QFT.

In relativistic QFT, the lowest-energy state cannot be annihilated by any observable that is strictly localized within in a finite region of space. This is a consequence of the **Reeh-Schlieder theorem**.[4] This implies that the first condition listed above (a detector observable should be local) is not strictly compatible with the third condition listed above (a detector shouldn't be triggered by the lowest-energy state). Relativistic QFT has local observables, and it has observables that annihilate the lowest-energy state, but it doesn't have any observables that satisfy both of those conditions.[5] That's okay, because the criteria are still approximately compatible with each other, and the quality of the approximation is consistent with the properties of real-world detectors.

Mathematically, we have two options: we can compromise the first criterion by allowing an observable that represents a detector to be only approximately localized, or we can compromise the third criterion by allowing a tiny but nonzero probability for the lowest-energy state to trigger a detector.[6,7] This article uses the first option: detectors that perfectly annihilate the vacuum state but that are only imperfectly localized.

Particles in the free scalar model are stable and don't interact with each other. In models that aren't this simple, attempts to define *particle* unambiguously can be frustrated by additional complications.[8] That's okay. Predictions should be unambiguous, but the ways we categorize predictions – like "this is a particle" or "this is a river" – don't need to be unambiguous.

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[4] Article 00980 briefly reviews the Reeh-Schlieder theorem, and section 2.4 in Witten (2018) highlights this particular consequence.

[5] Strictly nonrelativistic QFT (article 15939) avoids this complication by redefining *localized*, as explained in article 00980.

[6] Real detectors are slightly noisy anyway.

[7] This might be one reason why some popular accounts of QFT tell stories about particles bubbling in and out of existence in the vacuum state. Such stories can help inspire curiosity about QFT, but they don't really contribute to a proper understanding of QFT.

[8] Sometimes scattering experiments exhibit a *resonance* in a special range of energies, and sometimes the resonance lasts long enough to warrant calling it an intermediate *particle*, but the line is arbitrary.

3 Review of the free scalar model

Article 52890 constructs a family of models of a single scalar quantum field. The *free* scalar field is a special case in which the equation of motion is linear. In that special case, article 00980 explains how to make the time-dependence of the field operators explicit.

The construction used in those articles treats space as a lattice. This is artificial, but it allows the field operators to be defined at individual points without causing any mathematical trouble. This article uses continuum-like notation, but the model is understood to be defined on a lattice – the "integrals" are understood to be discrete sums. This section reviews some of the key equations from article 00980.

The field operators in the free scalar model may be written

$$\phi(\mathbf{x},t) = \int \frac{d^D p}{(2\pi)^D} \, \frac{a(\mathbf{p})e^{-i\omega t + i\mathbf{p}\cdot\mathbf{x}} + a^\dagger(\mathbf{p})e^{i\omega t - i\mathbf{p}\cdot\mathbf{x}}}{\sqrt{2\omega}} \tag{1}$$

with

$$[a(\mathbf{p}), a(\mathbf{p}')] = 0 \qquad\qquad [a(\mathbf{p}), a^\dagger(\mathbf{p}')] = (2\pi)^D \, \delta(\mathbf{p}' - \mathbf{p}) \tag{2}$$

and

$$\omega(\mathbf{p}) \approx \sqrt{m^2 + \mathbf{p}^2} \tag{3}$$

The approximation applies whenever $|\mathbf{p}|$ is much smaller than $1/\epsilon$, where ϵ is the lattice step-size.[9] In other words, the approximation applies whenever the resolution is coarse enough that the lattice might as well be a continuum. Section 11 shows that $\omega(\mathbf{p})$ is the energy of a particle with momentum $\mathbf{p}$, so equation (3) is the familiar Lorentz-symmetric relationship between energy, mass, and momentum (article 77597).

By definition, the field operator $\phi(\mathbf{x},t)$ is localized at $\mathbf{x}$ at time t, and any other observable qualifies as being localized in a spatial region R at time t if and only if it can be expressed in terms of operators $\phi(\mathbf{x},t)$ and $\dot{\phi}(\mathbf{x},t)$ with $\mathbf{x} \in R$. Equations (1)-(2) imply that the field operators satisfy these equal-time commutation

[9] This article uses natural units, in which Planck's constant $\hbar$ and the speed of light c are both equal to 1.

relations:

$$\big[\phi(\mathbf{x},t),\phi(\mathbf{y},t)\big]=0 \qquad\qquad \big[\dot\phi(\mathbf{x},t),\dot\phi(\mathbf{y},t)\big]=0$$
$$\big[\phi(\mathbf{x},t),\dot\phi(\mathbf{y},t)\big]=i\delta(\mathbf{x}-\mathbf{y}). \tag{4}$$

These can be used to test statements about the localization of other observables, because if an observable is localized in a region R at time t, then it must commute with $\phi(\mathbf{x},t)$ and $\dot\phi(\mathbf{x},t)$ for all points $\mathbf{x}$ that are not in R.

The hamiltonian for the free scalar model is

$$H=\int\frac{d^Dp}{(2\pi)^D}\;\omega(\mathbf{p})\,a^\dagger(\mathbf{p})a(\mathbf{p}). \tag{5}$$

The hamiltonian is the generator of translations in time, and it is the observable corresponding to the system's total energy. Saying that it generates translations in time means

$$\phi(\mathbf{x},t)=U^{-1}(t)\phi(\mathbf{x},0)U(t) \qquad\qquad U(t)\equiv e^{-iHt}.$$

To confirm that this is consistent with equations (1)-(2), use the commutation relations (2) to get $[a(\mathbf{p}),H]=\omega(\mathbf{p})a(\mathbf{p})$, which is the time-derivative of

$$U^{-1}(t)a(\mathbf{p})U(t)=a(\mathbf{p})e^{-i\omega(\mathbf{p})t}.$$

For each $\mathbf{p}$, the integrand of (5) is a positive operator, so the state $|0\rangle$ that satisfies

$$a(\mathbf{p})|0\rangle=0 \qquad\qquad \text{for all } \mathbf{p} \tag{6}$$

has the lowest possible energy. This is the vacuum state for the free scalar model. The Hilbert space is spanned by states of the form

$$a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2)\cdots a^\dagger(\mathbf{p}_N)|0\rangle$$

with $N\in\{0,1,2,...\}$.

4 Energy-increasing/decreasing operators

Equations (2) and (5) imply that each application of $a(\mathbf{p})$ decreases the energy of a state by $\omega(\mathbf{p})$. Its adjoint $a^\dagger(\mathbf{p})$ does the opposite: each application of $a^\dagger(\mathbf{p})$ increases the energy by $\omega(\mathbf{p})$. As promised by the Reeh-Schlieder theorem,[10] an operator that decreases the energy of every state cannot be strictly localized in any finite region of space. The identity

$$[a(\mathbf{p}), \phi(\mathbf{x}, t)] = \frac{e^{i\omega(\mathbf{p})t - i\mathbf{p}\cdot\mathbf{x}}}{\sqrt{2\omega(\mathbf{p})}}$$

shows that the operators $a(\mathbf{p})$ are not even close to being localized anywhere: the magnitude of the right-hand side is independent of $\mathbf{x}$.

An energy-decreasing operator can't be strictly localized in any finite region, but it can be approximately localized. The energy-decreasing operator defined by

$$a(\mathbf{x}, t) \equiv \int \frac{d^D p}{(2\pi)^D}\, a(\mathbf{p}) e^{-i\omega(\mathbf{p})t + i\mathbf{p}\cdot\mathbf{x}} = e^{iHt} a(\mathbf{x}, 0) e^{-iHt} \tag{7}$$

is *almost* localized at $\mathbf{x}$ at time t. This can be confirmed by using equation (1) to write $a(\mathbf{p})$ in terms of $\phi(\mathbf{y}, t)$ and $\dot\phi(\mathbf{y}, t)$[10] and observing that the coefficients of those field operators in $a(\mathbf{x}, t)$ are rapidly decreasing functions of $|\mathbf{x} - \mathbf{y}|$. It can also be checked by evaluating the commutators

$$[a(\mathbf{x}, t), \phi(\mathbf{y}, t)] = \int \frac{d^D p}{(2\pi)^D}\, \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\sqrt{2\omega(\mathbf{p})}}$$

$$[a(\mathbf{x}, t), \dot\phi(\mathbf{y}, t)] = i \int \frac{d^D p}{(2\pi)^D}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \sqrt{\omega(\mathbf{p})/2}.$$

Article 22050 shows that these are both rapidly decreasing functions of $|\mathbf{x} - \mathbf{y}|$.

[10] Article 00980

5 Detectors: construction

This section constructs a family of observables that act like detectors. Each detector is (approximately) localized in a specified region of space at time $t = 0$. Each of these observables is represented by a projection operator that perfectly annihilates the lowest-energy state, but they are only approximately localized (section 6).

The commutation relations (2) imply that the operators defined in (7) satisfy

$$\big[a(\mathbf{x},t),\, a(\mathbf{y},t)\big] = 0 \qquad\qquad \big[a(\mathbf{x},t),\, a^\dagger(\mathbf{y},t)\big] = \delta(\mathbf{x}-\mathbf{y}) \tag{8}$$

and

$$[a(\mathbf{p}), a^\dagger(\mathbf{x},t)] = e^{i\omega(\mathbf{p})t - i\mathbf{p}\cdot\mathbf{x}}. \tag{9}$$

For any given time t, the set of all linear combinations of state-vectors of the form

$$|\mathbf{x}_1,\, \mathbf{x}_2,\, ...,\, \mathbf{x}_N,\, t\rangle \equiv a^\dagger(\mathbf{x}_1,t)a^\dagger(\mathbf{x}_2,t)\cdots a^\dagger(\mathbf{x}_N,t)|0\rangle \qquad \text{with } N \in \{0,1,2,3,...\} \tag{10}$$

is **dense** in the Hilbert space: every nonzero vector in the Hilbert space has a nonzero inner product with at least one of these. If we specify an operator's effect on all of these state-vectors, then we have implicitly specified its effect on every state-vector in the Hilbert space.

Thanks to (8), the states (10) are mutually orthogonal, so we can define a projection operator $P(R,t)$ for each region R of space and each time t by

$$P(R,t)|\mathbf{x}_1,\, \mathbf{x}_2,\, ...,\, \mathbf{x}_N,\, t\rangle = \begin{cases} |\mathbf{x}_1,\, \mathbf{x}_2,\, ...,\, \mathbf{x}_N,\, t\rangle & \text{if at least one } \mathbf{x}_n \in R, \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Many other families of observables that act like imperfectly-localized detectors can also be constructed, but thanks to equations (8), the one defined here is especially easy to handle.

6 How localized are the detectors?

Remember (section 3) that an observable qualifies as being localized in a spatial region R at time t if and only if it can be expressed in terms of operators $\phi(\mathbf{x},t)$ and $\dot{\phi}(\mathbf{x},t)$ with $\mathbf{x}\in R$. According to that principle, the observables $P(R,t)$ defined in the previous section are not quite localized in R at time t. In fact, they're not quite localized in *any* finite region.

To prove this, first use the identity (9) to get

$$\begin{aligned}\langle 0|\phi(\mathbf{y},t)a^\dagger(\mathbf{x},t)|0\rangle &= \langle 0|\big[\phi(\mathbf{y},t),\, a^\dagger(\mathbf{x},t)\big]|0\rangle && \text{(use (6))}\\ &= \langle 0|0\rangle\, f_{1/2}(\mathbf{x}-\mathbf{y}) && \text{(use (9))}\end{aligned}$$

with

$$f_{1/2}(\mathbf{x}-\mathbf{y}) \equiv \int \frac{d^Dp}{(2\pi)^D}\,\frac{e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{x})}}{\sqrt{2\omega(\mathbf{p})}}. \tag{12}$$

The definition (11) gives

$$\langle 0|\phi(\mathbf{y},t)P(R,t)a^\dagger(\mathbf{x},t)|0\rangle = \langle 0|\phi(\mathbf{y},t)a^\dagger(\mathbf{x},t)|0\rangle \qquad \text{if } \mathbf{x}\in R \tag{13}$$

$$\langle 0|P(R,t)\phi(\mathbf{y},t)a^\dagger(\mathbf{x},t)|0\rangle = 0, \tag{14}$$

because $P(R,t)|0\rangle = 0$. Now, suppose (incorrectly) that $P(R,t)$ were localized in a finite region of space at time t, and let $\mathbf{y}$ be a point outside of that region. If that were true, then equations (4) would imply that $P(R,t)$ commutes with $\phi(\mathbf{y},t)$, so if $\mathbf{x}\in R$, then the quantities (13) and (14) would be equal to each other. That contradicts the fact that (12) is nonzero, so $P(R,t)$ cannot be localized in any finite region of space at time t.

On the other hand, the magnitude of the quantity (12) does decrease rapidly as $|\mathbf{x}-\mathbf{y}|$ increases,[11] so this result is consistent with the idea that $P(R,t)$ is *approximately* localized in R at time t.

[11] Article 22050

7 Single-particle states

Now that we've constructed some observables representing approximately localized detectors, we can use the ideas listed in section 2 to discover which states qualify as single-particle states. The observable $P(R,t)$ defined by equation (11) is a projection operator, so the probability that this detector will detect something in a state $|\psi\rangle$ is[12]

$$p_{|\psi\rangle}(R,t) \equiv \frac{\langle\psi|P(R,t)|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{15}$$

The lowest-energy state $|0\rangle$ doesn't have any particles, by definition. That's consistent with the identity

$$P(R,t)|0\rangle = 0,$$

which implies $p_{|0\rangle}(R,t) = 0$. Now consider the state

$$|\mathbf{x},t\rangle \equiv a^\dagger(\mathbf{x},t)|0\rangle. \tag{16}$$

This state satisfies

$$p_{|\mathbf{x},t\rangle}(R,t) = \begin{cases} 1 & \text{if } \mathbf{x} \in R, \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

It also satisfies

$$P(R,t)P(R',t)|\mathbf{x},t'\rangle = 0$$

for all R, R' with $R \cap R' = \varnothing$, for all times t and t' (not necessarily equal). According to the ideas listed in section 2, this means that the state (16) qualifies as a single-particle state, and equation (17) says that the particle is essentially localized in R at time t.

Any superposition (linear combination) of single-particle states is still a single-particle state, even though the particle in such a state might not be approximately

[12] Article 03431

localized in any small region of space. Any superposition of the states (16) may be written

$$|f,t\rangle \equiv \int d^D x \; f(\mathbf{x}) a^\dagger(\mathbf{x},t)|0\rangle. \tag{18}$$

This state doesn't (ever) have any more than one particle, because it does not trigger any pair of well-separated detectors, at any time t':

$$P(R,t')P(R',t')|f,t\rangle = 0$$

for all R, R' with $R \cap R' = \varnothing$. To confirm that the state (always) has at least one particle, choose a region R that is large enough to contain the region where f is nonzero. If needed, we can even choose R to be all of space. Using the notation (15), this ensures $p_{|f,t\rangle}(R,t) = 1$, so the state is guaranteed to trigger the detector $P(R,t)$. If the region R only partly overlaps the region where f is nonzero, then the detection probability will be less than 1. That's okay, because the criteria for diagnosing single-particleness don't require the particle to be detectable everywhere. They only require it to be detectable somewhere – not at any one point (section 8), but within some sufficiently large region.

8 How localized is the particle?

The state (16) represents a particle that is only imperfectly localized near $\mathbf{x}$ at time t. Equation (17) doesn't say that the particle is perfectly localized, because the observables $P(R,t)$ are not perfectly localized (section 6). We shouldn't expect perfect localization of any object to be possible anyway, because even the vacuum state is entangled with respect to location.[13] This section checks directly that the particle represented by the state (16) is only imperfectly localized.

If it were perfectly localized at $\mathbf{x}$, with no presence anywhere else, then the state $|\mathbf{x},t\rangle$ would look just like the vacuum state to all observables localized away from $\mathbf{x}$ at time t. More explicitly, the two quantities

$$\frac{\langle \mathbf{x},t|A|\mathbf{x},t\rangle}{\langle \mathbf{x},t|\mathbf{x},t\rangle} \qquad\qquad \frac{\langle 0|A|0\rangle}{\langle 0|0\rangle} \tag{19}$$

would be equal to eacy other for all observables $A \in \Omega(R,t)$ with $\mathbf{x} \notin R$, where $\Omega(R,t)$ is the set of observables localized in R at time t. But the two quantities (19) are *not* equal to each other for all such observables. To confirm this, write the first quantity as

$$\begin{aligned}
\frac{\langle \mathbf{x},t|A|\mathbf{x},t\rangle}{\langle \mathbf{x},t|\mathbf{x},t\rangle} &= \frac{\langle 0|a(\mathbf{x},t)Aa^\dagger(\mathbf{x},t)|0\rangle}{\langle 0|a(\mathbf{x},t)a^\dagger(\mathbf{x},t)|0\rangle} \\
&= \frac{\langle 0|[a(\mathbf{x},t),A]a^\dagger(\mathbf{x},t)|0\rangle + \langle 0|Aa(\mathbf{x},t)a^\dagger(\mathbf{x},t)|0\rangle}{\langle 0|a(\mathbf{x},t)a^\dagger(\mathbf{x},t)|0\rangle} \\
&= \frac{\langle 0|[a(\mathbf{x},t),A]a^\dagger(\mathbf{x},t)|0\rangle + \langle 0|A[a(\mathbf{x},t),a^\dagger(\mathbf{x},t)]|0\rangle}{\langle 0|[a(\mathbf{x},t),a^\dagger(\mathbf{x},t)]|0\rangle} \\
&= \frac{\langle 0|[a(\mathbf{x},t),A]a^\dagger(\mathbf{x},t)|0\rangle}{\langle 0|0\rangle\,[a(\mathbf{x},t),a^\dagger(\mathbf{x},t)]} + \frac{\langle 0|A|0\rangle}{\langle 0|0\rangle}.
\end{aligned}$$

This shows that the two quantities (19) cannot be equal to each unless the quantity

$$\langle 0|[a(\mathbf{x},t),A]a^\dagger(\mathbf{x},t)|0\rangle$$

[13] Article 00980

were zero for all $A \in \Omega(R,t)$ with $\mathbf{x} \notin R$. One example that makes it nonzero is

$$A = \phi^2(f)/2 \qquad\qquad \phi(f) \equiv \int d^D y \; f(\mathbf{y})\phi(\mathbf{y},t)$$

for some real-valued function f whose value at the point $\mathbf{x}$ is zero. Then

$$\begin{aligned}
\langle 0|[a(\mathbf{x},t), A]a^\dagger(\mathbf{x},t)|0\rangle &= \langle 0|[a(\mathbf{x},t), \phi(f)]\phi(f)a^\dagger(\mathbf{x},t)|0\rangle \\
&= \langle 0|[a(\mathbf{x},t), \phi(f)][\phi(f), a^\dagger(\mathbf{x},t)]|0\rangle \\
&= \langle 0|0\rangle \big|[a(\mathbf{x},t), \phi(f)]\big|^2 \\
&= \langle 0|0\rangle \left| \int \frac{d^D p}{(2\pi)^D} \int d^D y \; \frac{f(\mathbf{y}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\sqrt{2\omega(\mathbf{p})}} \right|^2 , \qquad (20)
\end{aligned}$$

which is nonzero even if f is zero at the point $\mathbf{x}$, as long as f is nonzero somewhere else. This shows that the particle represented by the state (16) is not perfectly localized at $\mathbf{x}$ (or anywhere else).[14]

On the other hand, the quantity (20) decreases rapidly with increasing distance between $\mathbf{x}$ and the region where f is nonzero. Explicitly, it decreases like $\sim \exp(-m|\mathbf{x}-\mathbf{y}|)$ where $\mathbf{y}$ is any point inside the region where f is nonzero.[15] This indicates that the particle is mostly (but still not perfectly) localized inside a region of diameter $\sim 1/m$, which is called the particle's **Compton wavelength**. This is consistent with the fact that the vacuum state's entanglement with respect to location decreases with increasing distance in essentially the same way.[16]

[14] Smit (2002), sections 2.8 and 2.9

[15] Article 22050

[16] Article 00980

9 Localized states: literature review

In quantum field theory, an association between observables and regions of spacetime is part of a model's definition.[17] The meaning of *localization* for a particle is therefore implicit in the way observables are used to define *particle*. That's the key message in section 8. More generally, the association between observables and regions of spacetime can be used as the foundation for the concept of *localization* for any type of state, whether or not the *particle* concept is involved. Such an observable-based definition of *localized state* is described in Knight (1961), who showed that it cannot be strictly satisfied by any state with a finite number of particles.[18] Licht (1963) derived a general result about the nature of operators that produce such states when applied to the vacuum state. The operators $a^\dagger(\mathbf{x}, t)$ defined in section 4 don't satisfy that condition, nor do any other operators that are constructed using only a finite number of factors of $a^\dagger(\mathbf{p})$.

A different (inequivalent!) way of defining *localization* for states was proposed earlier in Newton and Wigner (1949). With their definition, the states (10) are strictly localized, because a translation in space through a sufficiently large finite distance makes the translated state orthogonal to the original one. That might seem like a natural condition to require, but section 8 showed that it doesn't quite agree with the meaning of *localization* that comes from the model's local observables.[19]

Language is arbitrary, of course. The real question here is how quantum field theory relates to the real world, not how the words should be defined. Now matter how we might prefer to use the word *localization*, the fact that the definition used in Newton and Wigner (1949) disagrees with the one that comes from local observables is a language-independent insight about how quantum field theory relates to the real world.

[17] This association is usually specified with the help of field operators, but the general principles are independent of the method (Haag (1996) and article 21916).

[18] Knight (1961) defines the *number of particles* as the number of factors of $a^\dagger(\mathbf{p})$ applied to the vacuum state, which is presumptuous. This definition used in this article is less presumptuous, but in the free scalar model, it turns out to agree with the definition used in Knight (1961).

[19] Fleming (1998) studies the relationship between the Newton-Wigner definition and the Reeh-Schlieder theorem.

10 Localization and causality

In classical field theory, the principle of *causality* says that the region in which the initial data for two solutions of the equation of motion differ from each other cannot grow faster than a finite maximum speed (usually called the speed of light).[20] In QFT, the principle of causality is usually expressed exclusively in terms of observables (article 21916), without referring to states at all, but the definition of *localization* used in Knight (1961) can be used to relate the principle to states: the region in which two states differ from each other, as defined using local observables as in Knight (1961), should not grow any faster than the speed of light.

On the other hand, one of the key messages in this article is that a particle cannot be strictly localized: any one-particle state can be immediately distinguished from the vacuum state by observables that are localized far away. This is a general consequence of the Reeh-Schlieder theorem, not limited to the free scalar model. Time evolution in the free scalar model can't change the number of particles, but time evolution in most other models *can* change the number of particles. How can this be consistent with causality, if creating a particle requires modifying the state immediately everywhere in space?

Part of the answer is that the principle of causality is a comparison: it compares the consequences of two different initial states, with the same unitary time translation operator applied to both of them. Two states at time $t > 0$ cannot differ from each other everywhere in space unless the corresponding states at time $t < 0$ already differed from each other everywhere in space. If the two states that we're comparing at $t > 0$ have different well-defined numbers of particles, then causality says that the initial states that led to those final states must have already differed from each other – at least slightly – everywhere in space. That isn't paradoxical at all.

The rest of the answer can be illustrated with an example. In the free scalar model, the field operator $\phi(\mathbf{x}, t)$ is self-adjoint, so the operator

$$\exp(i\beta\phi(\mathbf{x}, t)) \tag{21}$$

[20] Article 98038

is unitary for any real number β. Applying this unitary operator to the vacuum state gives

$$|\beta\rangle = \exp\big(i\beta\phi(\mathbf{x},t)\big)|0\rangle. \tag{22}$$

In this state, the number of particles is undefined according to the detectors that were constructed in section 5. If β is small, then $|\beta\rangle$ is almost the same as the vacuum state, but with a small admixture of single-particle terms, an even smaller admixture of two-particle terms, and so on. An N-particle state cannot be strictly localized, but the state $|\beta\rangle$ is strictly localized: it can't be distinguished from the vacuum state by any observable A localized in a region that doesn't contain the point $\mathbf{x}$ at time t.[21] The proof is easy: A commutes with $\phi(\mathbf{x},t)$, and the operator (21) is unitary, so $\langle\beta|A|\beta\rangle = \langle 0|A|0\rangle$. The principle of causality says that if two states are initially differ from each other only within a finite region of space (according to local observables), then they can't ever differ from each other everywhere in space, so they can't end up with two different strictly well-defined numbers of particles. But most states don't have any strictly well-defined number of particles anyway – unless we project the final state onto a term with a well-defined number of particles, like we do when making probabilistic predictions about the outcome of a scattering experiment (article 03431).

Here's a less enlightening but more concise argument: the principle of causality is used in the proof of the Reeh-Schlieder theorem, and the Reeh-Schlieder theorem in turn implies that individual particles can't be strictly localized in the sense defined by local observables. This shows that causality is automatically consistent with the nonlocal nature of particles, even though they might seem to contradict each other at first glance.

[21] Here, I'm using the word *localized* the way Knight (1961) uses it.

11 The mass of a single particle

Now that we've identified the single-particle states, we can calculate the mass of a single particle. It turns out to be equal to the parameter m in the hamiltonian (5).[22]

By definition, the mass of a particle is just its energy when its momentum is zero.[23] In a model with Lorentz symmetry, we can express this in a momentum-independent way as (article 77597)

$$(\text{mass})^2 = (\text{energy})^2 - (\text{momentum})^2 \qquad \text{mass} \geq 0. \tag{23}$$

To use this definition, we need to know which observables represent energy and momentum. The energy operator is the hamiltonian (5), the generator of translations in time. The momentum operator should be the generator of translations in space. The usual concept of *generator* is not strictly valid when space is treated as a lattice, but we can still use it as an approximation at coarse resolution (compared to the lattice step-size ϵ), or equivalently at low energy (compared to $1/\epsilon$).[24] Article 00980 showed that the effects of a unitary translation operator $U(\delta\mathbf{x})$ on the operator $a(\mathbf{p})$ and the state $|0\rangle$ are

$$U^{-1}(\delta\mathbf{x})a(\mathbf{p})U(\delta\mathbf{x}) = a(\mathbf{p})e^{i\mathbf{p}\cdot\delta\mathbf{x}} \qquad U(\delta\mathbf{x})|0\rangle. \tag{24}$$

If space were continuous, we would define the generators of translations in space to be operators $\mathbf{P} = (P_1, P_2, ..., P_D)$ for which $U(\delta\mathbf{x}) = e^{i\mathbf{P}\cdot\delta\mathbf{x}}$. For infinitesimal $\delta\mathbf{x}$, equations (24) would become

$$[a(\mathbf{p}),\, \mathbf{P}] = \mathbf{p}\, a(\mathbf{p}) \qquad \mathbf{P}|0\rangle = 0. \tag{25}$$

[22] Warning: this is a special feature of the *free* scalar model. In models with interactions (nonlinear equations of motion), the relationship between a particle's mass and the parameters in the hamiltonian is usually not so simple.

[23] This statement uses natural units, in which the speed of light c is equal to 1. In standard international units, the mass is proportional to the rest-energy, with a factor of c^2 to convert between mass units and energy units.

[24] Article 00980 explains how the coarse-resolution condition can be expressed mathematically and why it's equivalent to low energy, at least for the free scalar model.

The conditions (25) are both satisfied by

$$\mathbf{P} = \int \frac{d^D p}{(2\pi)^D}\ \mathbf{p}\, a^\dagger(\mathbf{p}) a(\mathbf{p}), \tag{26}$$

so we can use the components of $\mathbf{P}$ as the momentum operators at resolutions that are coarse compared to ϵ. Now equation (23) says that the mass operator M should satisfy[25]

$$M^2 \equiv H^2 - \mathbf{P}^2 \qquad\qquad M \geq 0. \tag{27}$$

Use equations (5) and (26) in (27) to get

$$M^2 = m^2 \left(\int \frac{d^D p}{(2\pi)^D}\ a^\dagger(\mathbf{p}) a(\mathbf{p}) \right)^2 .$$

The operator in large parentheses is a positive operator (its spectrum is nonnegative), so we can take its square root to get

$$M = m \int \frac{d^D p}{(2\pi)^D}\ a^\dagger(\mathbf{p}) a(\mathbf{p}),$$

with the sign chosen to enforce the condition mass ≥ 0.

Now we can calculate the mass of any of the single-particle states (18). Use the identity (9) to get

$$M|f,t\rangle = m|f,t\rangle$$

with $|f,t\rangle$ given by (18). This shows that the parameter m in the hamiltonian is the mass of a single particle.[26]

[25] For an operator M, the condition $M \geq 0$ means that the spectrum of M should be nonnegative.

[26] Most of the single-particle states (18) don't have any strictly well-defined energy or momentum, because they are not eigenstates of the operators H or $\mathbf{P}$, but they all have a strictly well-defined mass m.

12 The motion of a single particle

Consider a single-particle state (18) that is approximately localized and that also has an approximately well-defined momentum $\mathbf{p}$. This section shows that the particle's location moves with velocity $\mathbf{p}/\omega(\mathbf{p})$, as expected from Lorentz symmetry.[27]

To show this, we can use an observable whose expectation value indicates the particle's location. Sections 7-8 showed that the state $a^\dagger(\mathbf{x},t)|0\rangle$ represents a single particle that is relatively well-localized at $\mathbf{x}$ at time t. Use the commutation relations (8) to confirm that the operators $\mathbf{X} = (X_1, ..., X_D)$ defined by

$$\mathbf{X}(t) = \int d^D x \; a^\dagger(\mathbf{x},t) a(\mathbf{x},t) \mathbf{x} \tag{28}$$

satisfy

$$\mathbf{X}(t)\, a^\dagger(\mathbf{x},t)|0\rangle = \mathbf{x}\, a^\dagger(\mathbf{x},t)|0\rangle.$$

This shows that within the space of single-particle states, we can use the operators $\mathbf{X}(t)$ as observables for the particle's location at time t,[28] so we can use $\dot{\mathbf{X}} \equiv d\mathbf{X}/dt$ as observables for the particle's velocity. Use the definition (7) in (28) to get

$$\dot{\mathbf{X}}(t) = \int \frac{d^D p}{(2\pi)^D} \int d^D x \; \big(i a^\dagger(\mathbf{p}) a(\mathbf{x},t) e^{i\omega(\mathbf{p})t - i\mathbf{p}\cdot\mathbf{x}} + \text{adjoint} \big) \omega(\mathbf{p}) \mathbf{x}, \tag{29}$$

where "adjoint" stands for the adjoint of the preceding term. To continue, treat $\mathbf{p}$ as a continuous quantity, which is a good approximation at resolutions much coarser than the lattice step-size ϵ. This gives

$$\int d^D x \; a(\mathbf{x},t) e^{-i\mathbf{p}\cdot\mathbf{x}} \mathbf{x} = i\nabla_{\mathbf{p}} \int d^D x \; a(\mathbf{x},t) e^{-i\mathbf{p}\cdot\mathbf{x}} = i\nabla_{\mathbf{p}} \big(a(\mathbf{p}) e^{-i\omega(\mathbf{p})t} \big)$$

[27] Article 77597

[28] The concept of a strict "position operator" doesn't make sense in relativistic QFT, because strict localization is not compatible with strict single-particleness, but a single particle can still have an *approximately* well-defined location. That's what the observables $\mathbf{X}(t)$ represent.

where $\nabla_{\mathbf{p}}$ is the gradient with respect to $\mathbf{p}$. Use this in the equation (29) to get

$$\begin{aligned}
\dot{\mathbf{X}}(t) &= -\int \frac{d^D p}{(2\pi)^D}\, \omega(\mathbf{p}) \Big(a^\dagger(\mathbf{p}) \nabla_{\mathbf{p}} \big(a(\mathbf{p}) e^{-i\omega(\mathbf{p})t} \big) e^{i\omega(\mathbf{p})t} + \text{adjoint} \Big) \\
&= -\int \frac{d^D p}{(2\pi)^D}\, \omega(\mathbf{p}) \left(a^\dagger(\mathbf{p}) \left(\nabla_{\mathbf{p}} a(\mathbf{p}) - i a(\mathbf{p}) \frac{\mathbf{p}}{\omega(\mathbf{p})} \right) + \text{adjoint} \right) \\
&= -\int \frac{d^D p}{(2\pi)^D}\, \omega(\mathbf{p}) \nabla_{\mathbf{p}} \big(a^\dagger(\mathbf{p}) a(\mathbf{p}) \big) \\
&= \int \frac{d^D p}{(2\pi)^D}\, a^\dagger(\mathbf{p}) a(\mathbf{p}) \nabla_{\mathbf{p}} \omega(\mathbf{p}) \\
&= \int \frac{d^D p}{(2\pi)^D}\, a^\dagger(\mathbf{p}) a(\mathbf{p}) \frac{\mathbf{p}}{\omega(\mathbf{p})}.
\end{aligned} \tag{30}$$

To apply this, consider a single-particle state (18) that is mostly localized at $\mathbf{x}_0$ at time $t = 0$ and that has a somewhat well-defined momentum $\mathbf{p}_0$. Example:

$$\begin{aligned}
|\psi\rangle &\equiv \int d^D x\; e^{-(\mathbf{x}-\mathbf{x}_0)^2/2\sigma^2} e^{i\mathbf{p}_0\cdot\mathbf{x}} a^\dagger(\mathbf{x}, 0)|0\rangle \\
&\propto \int \frac{d^D p}{(2\pi)^D}\; e^{-(\mathbf{p}-\mathbf{p}_0)^2\sigma^2/2} e^{i\mathbf{p}\cdot\mathbf{x}_0} a^\dagger(\mathbf{p})|0\rangle,
\end{aligned}$$

where σ is a real parameter. This is a single-particle state with width $\sim \sigma$ in the spatial domain and $\sim 1/\sigma$ in the momentum domain. By inspection, the expectation values of $\mathbf{X}(0)$ and $\mathbf{P}$ in this state are

$$\frac{\langle\psi|\mathbf{X}(0)|\psi\rangle}{\langle\psi|\psi\rangle} = \mathbf{x}_0 \qquad\qquad \frac{\langle\psi|\mathbf{P}|\psi\rangle}{\langle\psi|\psi\rangle} = \mathbf{p}_0,$$

and equation (30) shows that the expectation value of $\dot{\mathbf{X}}(t)$ is

$$\frac{\langle\psi|\dot{\mathbf{X}}(t)|\psi\rangle}{\langle\psi|\psi\rangle} \approx \frac{\mathbf{p}_0}{\omega(\mathbf{p}_0)}. \tag{31}$$

This completes the derivation.

13 Multi-particle states

In the free scalar model, according to the ideas listed in section 2, a state of the form

$$|\psi\rangle = a^\dagger(\mathbf{x}_1, 0)a^\dagger(\mathbf{x}_2, 0)\cdots a^\dagger(\mathbf{x}_N, 0)|0\rangle \tag{32}$$

is an N-particle state. It doesn't have any more than N particles, because the commutation relations (8) imply that such a state satisfies

$$\left(\prod_k P(R_k, t_k)\right)|\psi\rangle = 0$$

for any list of more than N non-overlapping regions R_k at any times t_k. If the N points $\mathbf{x}_n$ are all separated, then we can choose N regions R_n, each of which contains just one of the points $\mathbf{x}_n$, to construct a coincidence arrangment of detectors that will all be triggered with certainty. Such a coincidence arrangement is represented by the observable $\prod_n P(R_n, 0)$. This shows that it is an N-particle state, at least if the points are separated.

Any superposition of N-particle states is still an N-particle state. We can use this to construct states in which the location and momentum of each particle are both somewhat well-defined, as in section 12. An example is

$$|\psi\rangle = C_1(0)C_2(0)\cdots C_N(0)|0\rangle \tag{33}$$

with

$$C_n(t) \equiv \int d^D x\ e^{-(\mathbf{x}-\mathbf{x}_n)^2/2\sigma^2} e^{i\mathbf{p}_n\cdot\mathbf{x}} a^\dagger(\mathbf{x}, t) = e^{iHt}C_n(0)e^{-iHt},$$

where $\mathbf{x}_n$ and $\mathbf{p}_n$ are the (approximately well-defined) location and momentum of a particle at time $t = 0$. In the Schrödinger picture, the state (33) evolves in time as

$$e^{-iHt}|\psi\rangle = C_1(t)C_2(t)\cdots C_N(t)|0\rangle.$$

From this, we can immediately infer that the particles don't interact with each other: each one behaves just as it would if the others were absent.[29,30] This gives us a good reason to call (32) an N-particle state even if two or more of the points $\mathbf{x}_n$ coincide.

In models with interactions, things are usually not so simple. In the free scalar model, the guidelines described in section 2 lead to a relatively straightforward relationship between particles and the energy increasing/decreasing parts of the field operators. In most models, the relationship between particles and the field operators is more complicated – so much so that it's usually intractable. And in most models, particles are transient phenomena: their number can change and usually isn't even well-defined at all. The guidelines described in section 2 can be used in any model, but they don't guarantee that the particle concept will make sense in all circumstances. It often doesn't, and accepting this fact removes one of the most common obstacles to a better understanding of QFT.

[29]This is why the free scalar model is called *free* or *non-interacting*.

[30]This result would not hold if the hamiltonian involved powers of ϕ higher than quadratic. For this reason, higher-than-quadratic terms in the hamiltonian are called **interaction terms**.

14 The nonrelativistic approximation

The nonrelativistic approximation is defined by the condition

$$(\text{momentum})^2 \ll (\text{mass})^2.$$

Equations (2) and (26) give

$$\mathbf{P}\, a^\dagger(\mathbf{p})|0\rangle = \mathbf{p}\, a(\mathbf{p})|0\rangle,$$

so for a single-particle state (18), the nonrelativistic approximation amounts to considering only superpositions of the states $a^\dagger(\mathbf{p})|0\rangle$ with $\mathbf{p}^2 \ll m^2$. In the context of such states, we can use this approximation for the quantity (3):

$$\omega(\mathbf{p}) \approx m + \frac{\mathbf{p}^2}{2m}.$$

Substitute this into (5) and use (7) to get this expression for the effective hamiltonian in the nonrelativistic approximation:

$$H \approx \int d^D x\; a^\dagger(\mathbf{x}, t) \left(m - \frac{\nabla^2}{2m} \right) a(\mathbf{x}, t).$$

This matches the no-interaction case of the nonrelativistic boson model constructed in article 15939.

15 Other ways to think about particles

The criteria described in section 2 are physically intuitive, but they're not always computationally convenient. A more convenient criterion uses the spectrum of the mass operator. Roughly, the idea is that when a model is defined in infinite volume so that the total momentum can be varied continuously, (normalizable) eigenstates of the mass operator are single-particle states.[31] To see why this makes sense, consider a state with two or more particles with zero total momentum. When the total momentum is zero, the mass is (by definition) proportional to the total energy. In a state with two or more particles, we can change the total energy continuously by changing the particles' relative velocities without changing the total momentum. This shows that a state with two or more particles cannot be an (normalizable) eigenstate of the mass operator, so eigenstates of the mass operator must be single-particle states.[32] This criterion doesn't work in all cases,[33] but when it works, it is convenient.

When it works, the mass-spectrum criterion has a nice implication: eigenvalues of the mass operator (with normalizable eigenstates) lead to poles in correlation functions. This is explained in most standard introductions to quantum field theory, because it's part of the justification for the usual approach to calculating scattering cross sections.[34]

Another way to think about particles is to use the representation theory of the Poincaré group. Here's the idea: for any given species of particle, the corresponding set of one-particle states is self-contained under linear combinations and also under the action of the (identity component of the) Poincaré group.[35] Conversely, if a set

[31] In a model with more than one superselection sector, this criterion can be applied separately in each sector.

[32] Enss (1975) gives a more detailed analysis of how the mass-spectrum criterion relates to the guidelines that were listed in section 2.

[33] It doesn't work nicely in models with massless particles. It also doesn't work nicely for massive particles that carry long-range charges, like electrostatic charges (Buchholz (1986)). In other words, it doesn't work nicely for most of the particles in the Standard Model! A large amount of literature has been written about how to work around this little inconvenience. Some of it can be found by searching online for the keyword *infraparticle*.

[34] Weinberg (1995), sections 10.2 and 10.3

[35] Transformations that aren't in the identity component, like a reflection along a single dimension of spacetime,

of single-particle states constitutes a reducible representation of the Poincaré group, then its irreducible components can be regarded as distinct species.[36] This leads to a coarse classification of particles according to irreducible unitary representations of the Poincaré group.[37]

Thse other ways of thinking about particles in QFT are already explained well in plenty of other sources, so I won't review them in any detail here.

might transform different species into each other.

[36]This makes sense because a reducible unitary representation (of any group) is completely reducible. Proof: let $\mathcal{H}_1$ be a subspace of the Hilbert space, and let $\mathcal{H}_2$ be its orthogonal complement. If $\mathcal{H}_1$ is self-contained under the action of the group, then $\langle 2|U|1\rangle = 0$ for every $|1\rangle \in \mathcal{H}_1$, every $|2\rangle \in \mathcal{H}_2$, and every U in the representation of the group. This implies $\langle 1|U^\dagger|2\rangle = 0$ for every $|1\rangle \in \mathcal{H}_1$, which implies $U^\dagger|2\rangle \in \mathcal{H}_2$. A unitary representation is self-contained under adjoints, so this implies that $\mathcal{H}_2$ is self-contained under the action of the group.

[37]Bekaert and Boulanger (2006)

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