Causality, particle localization and positivity of the energy

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Abstract

Positivity of the Hamiltonian alone is used to show that particles, if initially localized in a finite region, immediately develop infinite tails.

1. Introduction

The concept of finite signal velocity or, more precisely, the speed of light as highest signal velocity is often called Einstein causality. If, in the special theory of relativity, there were superluminal signals then there could exist tachyons, i.e. superluminal particles, and the sequence of cause and effect could be reversed. On the other hand, if signals of arbitrarily high velocities existed, one could also argue that one could obtain absolute clock synchronization and absolute simultaneity, thus making a revision of special relativity necessary.

In usual quantum mechanics it is well known that wave functions, if initially localized in a finite region, immediately develop infinite tails. For a nonrelativistic theory this is of no concern. A similar phenomenon was then noted, however, for the Newton-Wigner position operator [1, 2, 3]. In fact, the question of localization in quantum field was recognized as a difficult problem quite early [4]. In particular, localization by means of a current-density four-vector were investigated in a class of models [5].

It was then recognized by the present author that the superluminal spreading had nothing to do with position operators, field equations, current densities or

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a particular notion of particle localization. In a model-independent way the theorem was proved that a free relativistic particle, if initially localized with probability 1 in a finite (bounded) region, immediately thereafter would have spread over all space [8]. An alternative proof of this theorem was given in [7] and a generalization to relativistic systems in [8]. The theorem was carried over to quite general interactions, not necessarily relativistic ones in [9]. It became apparent in that paper that the main ingredient was positivity of the energy, with translation invariance used as a technical tool.

In 1985 the present author [10] showed that the connection between localization and Einstein causality was more restrictive than previously thought. It was proved in [10] that relativistic systems with Gaussian-like bounded tails at \( t = 0 \) – provided they exist! – would lead to a superluminal probability flow.

The main purpose of this paper is to show that translation invariance is not needed for superluminal spreading of particles which are initially confined in a bounded region. For this purpose a recent result [11] of the present author for Fermi’s two-atom system will be reformulated in Section 2 as an abstract mathematical theorem and applied to particle localization. It will then be shown that, as a consequence of positivity of the energy alone, a particle which is initially strictly localized in a finite region either stays there indefinitely or immediately develops infinite tails. In the last section the connection to Einstein causality is discussed. As in the author’s result [11] on the Fermi problem several ways out are mentioned to avoid a conflict.

### 2. A consequence of positivity of the energy

In this section we will prove a simple mathematical result on the temporal behavior of certain expectation values. If the time-development operator is positive one might expect analyticity properties, but for arbitrary expectation values this is not true. One has, however, the following result.

**Theorem:** Let \( H \) be a selfadjoint operator, positive or bounded from below, in a Hilbert space \( \mathcal{H} \). For given \( \psi_0 \in \mathcal{H} \) let \( \psi_t, t \in \mathbb{R} \), be defined as

\[
\psi_t = e^{-iHt}\psi_0.
\]

(1)

Let \( A \) be a positive operator in \( \mathcal{H} \), \( A \geq 0 \), and let \( p_A(t) \) be defined as

\[
p_A(t) = \langle \psi_t, A\psi_t \rangle.
\]

(2)

Then either

\[
p_A(t) \neq 0 \quad \text{for almost all} \quad t
\]

(3)
and the set of such \( t \)'s is dense and open, or

\[
p_A(t) \equiv 0 \quad \text{for all } \ t.
\]  

(4)

The proof is based on an analyticity argument for which, however, a little care – and the positivity of \( A \) – is needed. Evidently, since \( H \geq -c \), one can define \( \exp\{-iH(t + iy)\} \) for \( y \leq 0 \), and \( \exp\{-iHz\} \) is analytic in \( z \) for \( \text{Im} \ z < 0 \), and hence \( \psi_t \) can be analytically continued to the lower half-plane, with continuous boundary values on the real axis. However, the r.h.s. of Eq. (2) can in general not be analytically continued since it equals

\[
\langle \psi, e^{iHt} A e^{-iHt} \psi \rangle
\]

and since \( \exp\{i(H + iy)t\} \) is in general unbounded for \( y < 0 \). To by-pass this the positivity of \( A \) can be used. We write

\[
p_A(t) = \langle A^{1/2} \psi_t, A^{1/2} \psi_t \rangle
\]  

(5)

where \( A^{1/2} \) is the positive square root of \( A \), and denote by \( \mathcal{N}_0 \) the set of \( t \)'s for which \( p_A(t) = 0 \). By continuity of \( p_A(t) \), \( \mathcal{N}_0 \) is closed and its complement \( \mathcal{N}_0^c \) is open. Eq. (5) now implies

\[
A^{1/2} \psi_t = 0 \quad \text{for } t \in \mathcal{N}_0.
\]  

(6)

For fixed \( \phi \in \mathcal{H} \) we define the function \( F_\phi(z) \) for \( \text{Im} \ z \leq 0 \) by

\[
F_\phi(z) = \langle \phi, A^{1/2} e^{-iHz} \psi_0 \rangle.
\]  

(7)

By the above remark on \( \exp\{-iHz\} \), \( F_\phi(z) \) is a continuous function for \( \text{Im} \ z \leq 0 \) and is analytic for \( \text{Im} \ z < 0 \). By Eq. (3) one has

\[
F_\phi(t) = 0 \quad \text{for } t \in \mathcal{N}_0.
\]  

(8)

Now let us assume that the complement \( \mathcal{N}_0^c \) is not dense. Then \( \mathcal{N}_0 \) contains some interval \( I \) of nonzero length, and \( F_\phi(z) \) vanishes on \( I \). One can now directly employ the Schwarz reflexion principle \[12\] to conclude that \( F_\phi(z) \equiv 0 \) or proceed in a more pedestrian way as follows. One defines an extension of \( F_\phi \) to the upper half plane by putting

\[
F_\phi(z) = F_\phi(z^*)^* \quad \text{for } \text{Im} \ z > 0.
\]  

(9)

Since \( F_\phi(t) = 0 \) for \( t \in I \) and thus, a fortiori, real for \( t \in I \), the extension \( F_\phi(z) \) continuous for \( z \in I \). From this one easily shows \[12\] that \( F_\phi(z) \) is analytic for \( z \notin \mathbb{R} \setminus I \), and thus \( I \) is contained in the domain of analyticity. Since \( F_\phi(z) \) vanishes on \( I \) it must therefore vanish on the analyticity domain, i.e. for \( z \notin \mathbb{R} \setminus I \).
By continuity $F_{\phi}(z)$ then vanishes everywhere. Since $\phi$ was arbitrary, we obtain $A^{1/2}\psi_z = 0$ for all $t$. Hence,

$$A\psi_t = 0 \quad \text{for all } t$$

and thus $p_A(t) \equiv 0$ if $\mathcal{N}_0^c$ is not dense, i.e. alternative (ii) holds in this case.

Since a dense open set need not have full Lebesgue measure, it remains to show that $\mathcal{N}_0$ is a null set if alternative (ii) does not hold. To prove this we use the fact that, as a boundary value of a bounded analytic function, $F_{\phi}(t)$ satisfies the inequality

$$\int_{-\infty}^{\infty} dt \ln|F_{\phi}(t)| \frac{1}{1 + t^2} > -\infty$$

unless it vanishes identically. If $\mathcal{N}_0$ had positive measure the integral would be $-\infty$, and thus $F_{\phi}(t)$ would vanish for all $t$, for each $\phi$. This would again imply alternative (ii). This proves the theorem.

The theorem is a more abstract version of a result in [11] on Fermi’s two-atom problem. To check the speed of light in quantum electrodynamics, Fermi had considered two atoms, separated by a distance $R$ and with no photons present initially. One of the atoms was assumed to be in its ground state, the other in an excited state. The latter could then decay with the emission of a photon. Fermi calculated the excitation probability of the atom which had initially been in its ground state. Using standard approximations he found the excitation probability to be zero for $t < R/c$.

Now, if one takes for $\psi_0$ in the theorem the initial state considered by Fermi and for $A$ the operator describing the excitation probability, e.g. the projector onto the excited states, then $p_A(t)$ becomes the excitation probability, and the theorem states that this probability is immediately nonzero. Already in [11] it was discussed how to avoid a possible conflict with causality, and this was continued in more detail for example in [14, 13, 16, 17]. The upshot was that the immediate excitation could be understood in a field-theoretic context through vacuum fluctuations due to virtual photons. The part of the excitation due to the second atom behaves causally [16, 17]. Causality then holds for expectation values after the spontaneous part has been subtracted. This corresponds to the notion of weak causality, i.e. for expectation values, introduced in [2], which contrasts to the notion of strong causality, i.e. causality for individual events, as discussed in [14]. Fermi seems to have had strong causality in mind.

3. Application to particle localization and spreading

We will now apply the above theorem to the question of particle localization.
We note that the results hold independent of whether the theory is relativistic or not, or a field theory or not. Neither is the existence of a position operator assumed. The ingredient is just positivity of the energy. Translation invariance, which was used in previous treatments \[6, 9, 10, 18\], is not needed here.

Let us suppose that it makes sense to speak of particles inside some volume \( V \), i.e. of the probability to find a particle at a given time in \( V \). This is a highly nontrivial assumption. Indeed, it has been argued \[19\] that in algebraic quantum field theory the notion of local particle states may make sense only asymptotically for free particles.

In a quantum theory the probability to find a particle or system inside \( V \) should be given by the expectation of an operator, \( N(V) \) say. Since probability lie between 0 and 1, one must have

\[
0 \leq N(V) \leq 1 . \tag{12}
\]

Now let us assume that the system, with state \( \psi_0 \) at \( t = 0 \), is strictly localized in a region \( V_0 \), i.e. with probability 1, so that

\[
\langle \psi_0, N(V_0) \psi_0 \rangle = 1 \tag{13}
\]
or, equivalently,

\[
\langle \psi_0, (1 - N(V_0)) \psi_0 \rangle = 0 . \tag{14}
\]

From Eq. (12) one has

\[
1 - N(V_0) \geq 0 \tag{15}
\]
and hence the theorem can be applied, with \( A \equiv 1 - N(V_0) \). As a consequence one either has

\[
\langle \psi_t, N(V_0) \psi_t \rangle \equiv 1 \for all \ t \tag{16}
\]
or

\[
\langle \psi_t, N(V_0) \psi_t \rangle < 1 \for almost all \ t . \tag{17}
\]

The argument in Eqs. (14-17) is for pure states. It can easily be carried over to mixtures characterized by density matrices. Eq. (13) is then replaced by

\[
tr(\rho_0 N(V_0)) = 1 . \tag{18}
\]
Writing

\[
\rho_0 = \sum \alpha_i | \psi_{i0} \rangle \langle \psi_{i0}| \tag{19}
\]
with \( \sum \alpha_i = 1 \), Eq. (18) becomes

\[
\sum_i \alpha_i \langle \psi_{i0}, N(V_0) \psi_{i0} \rangle = 1
\]
which implies

\[
\langle \psi_{i0}, N(V_0) \psi_{i0} \rangle = 1 \for all \ i .
\]
Then one can proceed as before and obtains that either

\[ tr(\rho_t N(V_0)) \equiv 1 \quad \text{for all } t \]  
\[ tr(\rho_t N(V_0)) < 1 \quad \text{for almost all } t . \]

Alternative (20) or (16) means that the particle or system stays in \( V_0 \) for all times, as might happen for a bound state in an external potential.

Now, if the particle or system is strictly localized in \( V_0 \) at \( t = 0 \) it is, a fortiori, also strictly localized in any larger region \( V \) containing \( V_0 \). If the boundaries of \( V \) and \( V_0 \) have a finite distance and if finite propagation speed holds then the probability to find the system in \( V \) must also be 1 for sufficiently small times, e.g. \( 0 \leq t < \epsilon \). But then the theorem, with \( A \equiv 1 - N(V) \), states that the system stays in \( V \) for all times. Now, we can make \( V \) smaller and let it approach \( V_0 \). Thus we conclude that if a particle or system is at time \( t = 0 \) strictly localized in a region \( V_0 \), then finite propagation speed implies that it stays in \( V_0 \) for all times and therefore prohibits motion to infinity. Or put conversely, if there exist particle states which are strictly localized in some finite region at \( t = 0 \) and later move towards infinity, then finite propagation speed cannot hold for localization of particles.

This can be formulated somewhat more strongly as follows. If at \( t = 0 \) a particle is strictly localized in a bounded region \( V_0 \) then, unless it remains in \( V_0 \) for all times, it cannot be strictly localized in a bounded region \( V \), however large, for any finite time interval thereafter, and the particle localization immediately develops infinite ‘tails’. The spreading is over all space except possibly for ‘holes’ which, if any, will persist for all times, by the same arguments as before. If the theory is translation invariant then there can be no holes, as shown in [9] under some mild spectrum conditions.

4. Discussion. Connection with causality

As shown above, a particle or system, if initially strictly localized in a bounded region, will immediately develop infinite tails except in the exceptional case that it stays in the original region for all times. The latter seems to require external potentials, and this will be disregarded here. If a particle is part of a larger system, e.g. of a composite system, the results still apply, and the appearance of immediate infinite tails may be attributed to the center-of-mass motion.

In nonrelativistic quantum mechanics the immediate spreading of wave functions over all space is a well known phenomenon. In a relativistic theory this might lead to a conflict with Einstein causality if it were observable. Indeed, if a particle were initially strictly localized in some region on earth and if there were a nonzero probability, however small, to observe the particle a fraction of a
second later on the moon, this could be used for the absolute synchronization of clocks. One simply would have repeat the experiment sufficiently often, preferably with distinguishable particles in order to be sure when a detected particle was originally released.

But isn’t the Dirac equation for a free particle of spin 1/2 a counterexample to our results? This is, however, not so. Indeed, the Dirac equation is hyperbolic and thus satisfies finite propagation speed. If for the localization operator $N(V)$ one takes the characteristic function $\chi_V(x)$ then, for a wave function with initial support in a finite region, the localization does evolve causally. However, the Dirac equation contains positive and negative energy states, and we therefore can conclude from our results that positive-energy solutions of the Dirac equation always have infinite support (cf. also [20]).

This example suggests a simple solution to the causality problem seemingly connected with particle localization. If there would not exist any particle states localized with probability 1 in a bounded region or, more generally, if all systems were spread out over all space to begin with, then no problems would arise. This would imply in particular that $N(V)$ could not have the eigenvalue 1 and thus could not be a projector. As a consequence there would be no selfadjoint position operator satisfying causal requirements, not even if one allowed position operators with noncommuting components as suggested, e.g., in [21]. For if one had a selfadjoint component of a position operator then its spectral decomposition would yield localization operators $N(V)$ for $V$’s being infinite slabs, and to these the results could be applied in the same way as to bounded regions.

If one adopts the standpoint that all particle states have infinite tails to begin with, one might also argue that these tails could be made to drop off as fast as one likes, thus approximating a strictly localized state to arbitrary accuracy. In [10] it was shown, however, that in a relativistic theory such tails cannot drop off arbitrarily fast.

In a field theoretic context the permanent infinite tails could be intuitively understood through clouds of virtual particles around real particles ("dressed particle states"). Sometimes it is simply argued that local commutation or anti-commutation relations of the fields must clearly ensure causal behavior of localized particles. This overlooks the possibility that the operator $N(V)$ – if it exists – might not be a local function of the fields. A more satisfactory discussion of causality aspects is given in algebraic quantum field theory in [2] and in an alternative algebraic framework in [22].

Instead of speaking about infinite tails one may also envisage that all particle detectors exhibit inherent noise due to vacuum fluctuations and that therefore localization with probability 1 or zero can never be recorded. This would essentially lead to the same conclusion as permanent infinite tails.

Finally, it may well be true that, as advocated in [19], the notion of localizable
particles in field theory makes sense only for free particles.

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