Causality, delocalization and positivity of energy.

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Abstract

In a series of interesting papers G. C. Hegerfeldt has shown that quantum systems
with positive energy initially localized in a finite region, immediately develop infinite
tails. In our paper Hegerfeldt’s theorem is analysed using quantum and classical wave
packets. We show that Hegerfeldt’s conclusion remains valid in classical physics. No
violation of Einstein’s causality is ever involved. Using only positive frequencies, complex
wave packets are constructed which at $t = 0$ are real and finitely localized and which,
furthermore, are superpositions of two nonlocal wave packets. The nonlocality is initially
cancelled by destructive interference. However this cancellation becomes incomplete at
arbitrary times immediately afterwards. In agreement with relativity the two nonlocal
wave packets move with the velocity of light, in opposite directions.
1 Introduction

Are there deviations from Einstein’s causality? G. C. Hegerfeldt has written [1]: “Positivity of the Hamiltonian alone is used to show that particles, if initially localized in a finite region, immediately develop infinite tails.” This seems to imply superluminality. One of his examples is the Fermi problem [2] of two atoms coupled by a radiation field. Consider the initial condition when one of the atoms is in an excited state, the other in the ground state, and no photons are present. The probability to find the second atom in an excited state is non-vanishing immediately after the initial moment, independently of the distance between the atoms [1], [3] - [5]. Hegerfeldt’s arguments are based on the analyticity of the expectation values of the operator $N(V)$, which gives the probability to find a particle inside a finite volume $V$. He showed that a state in a quantum system with positive energy localized in a finite volume $V$ at the instant $t = 0$, will develop infinite tails immediately afterwards. Positivity of energy plays an essential role in his proof. In this paper we present an illustration of Hegerfeldt’s theorem, without any appeal to superluminality. We apply Hegerfeldt’s consideration to wave packets. Moreover, we show that Hegerfeldt’s effect appears even for classical fields, if wave packets are constructed from positive frequencies (corresponding positive energy quantum fields).

We first study the positive-frequency solutions of the classical wave equation (section 2). We consider wave packets $\Phi(x,t)$ localized at $t = 0$. The localization is due to interference of the two complex solutions, each propagating causally

$$\Phi(x,t) = \psi(x-t) + \psi^*(x+t)$$

where "*" denotes complex conjugation and we take $c = 1$. We show that both these wave packets are delocalized. They present long tails, extending to arbitrary distances and decaying according to a power law. As we shall show, the “nonlocal effect” can also be understood from the point of view of the initial conditions. Indeed, in our construction of the solution [1] we shall use two conditions; one is the initial condition of the local
shape of the field $\Phi(x, t)$ and the other is the condition of the positivity of frequencies. The frequency positivity replaces the usual initial condition on the time derivative of the field $\partial \Phi / \partial t$. We shall show that our initial condition with positive frequencies leads to the nonlocality of $\partial \Phi / \partial t$ at $t = 0$.

In section 3 we show that similar conclusions are obtained for the wave packet of a free field in relativistic quantum field theory. We construct an operator reminding of the position operator of Newton-Wigner [6]. The expectation value of this operator with the state corresponding to our wave packet is local at $t = 0$. However, it has infinite tails which are “hidden” at time $t = 0$, but emerge immediately afterwards. We may call this effect a “curtain” effect. No superluminal propagation is involved. We note that at the same time other quantities such as the energy density have a nonlocal expectation value in the same state even for $t = 0$. It should be also pointed out that for the Dirac equation there are no positive energy solutions which can be localized in a finite region (see [4]). This demonstrates that localization in relativistic quantum field theory cannot be “complete”.

2 Classical wave packets

Consider classical wave packets constructed by the solutions of the wave equation with positive frequency and localized at time $t = 0$. We show that these wave packets will spread immediately over the whole space. Curiously we have not found any reference to this effect in the literature. We start from the wave equation on the real line ($c = 1$).

$$\left( \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) \Phi(x, t) = 0 \quad (2)$$

The general complex solution of Eq. (2) is, by the Fourier transform, of the form

$$\Phi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left\{ \phi_+(k)e^{-i\omega k t} + \phi_-(k)e^{i\omega k t} \right\} e^{ikx} \quad (3)$$
where \( \omega_k = |k| \) and where \( \phi_{\pm}(k) \) are arbitrary functions. To determine \( \phi_+ \) and \( \phi_- \) one can use the two initial conditions \( \Phi(x,0) \) and \( \dot{\Phi}(x,0) \). However, one can also consider the special class of positive-frequency solutions to Eq. (2), i.e. \( \phi_-(k) \equiv 0 \) and

\[
\Phi_+(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \phi_+(k) e^{-i\omega_k t} e^{ikx} \tag{4}
\]

These positive-frequency solutions are determined by the initial condition \( \Phi(x,0) \). Note that relation (3) leads to a complex field for \( t \neq 0 \), even if \( \Phi_+(x,0) \) or \( \phi_+(k) \) are real.

Consider as an example a localized (rectangular) wave packet with center \( x_0 \), and width \( 2b \) at time \( t = 0 \):

\[
\Phi_{x_0,b}(0) = \frac{1}{2b} \Theta(b - |x - x_0|) \tag{5}
\]

The normalization has been chosen so that the integral of this function over \( x \) is equal to one. Then the function \( \phi(k) \) is:

\[
\phi_+(k) = \frac{1}{2b} \int_{-\infty}^{\infty} dx e^{-ikx} \Theta(b - |x - x_0|) \tag{6}
\]

where \( \Theta(x) \) is the step function, which is 0 for \( x \) negative, and 1 for \( x \) positive. Then the function \( \Phi(x,t) \) in (3) is given by

\[
\Phi(x,t) = \frac{1}{4\pi b} \int_{-\infty}^{+\infty} dk \int_{x_0-b}^{x_0+b} dx' e^{-i|k|t+ik(x-x')} \tag{7}
\]

This is a sum of two functions corresponding to two wave packets moving in opposite directions,

\[
\Phi(x,t) = \psi(x-t) + \psi^*(x+t) \tag{8}
\]

where

\[
\psi(x) = \frac{1}{4\pi b} \int_{x_0-b}^{x_0+b} dx' \int_{0}^{+\infty} dk e^{ik(x-x')} \tag{9}
\]

To evaluate the integral over \( k \) we introduce the usual regularisation by adding a positive infinitesimal to \( x \), which leads to

\[
\psi(x) = -\frac{1}{4\pi bi} \int_{x_0-b}^{x_0+b} dx' \frac{dx'}{x-x'+i0} \tag{10}
\]
After integration over $x'$ we obtain:

$$\psi(x) = \frac{i}{4\pi b} [\ln(x - x_0 + b + i0) - \ln(x - x_0 - b + i0)]$$  \hspace{1cm} (11)

The logarithm of a complex number is given by

$$\ln(z) = \ln|z| + i(\text{arg}(z) + 2\pi n)$$  \hspace{1cm} (12)

where $n$ is an integer. In order to have both terms in (11) on the same branch of the logarithm we take $n = 0$ for both of them (due to the difference of the two terms in (11) the result does not depend on the particular value of $n$). The argument of $x + i0$ can be expressed as

$$\text{arg}(x + i0) = \frac{\pi}{2} (1 - \text{sign}(x))$$  \hspace{1cm} (13)

where $\text{sign}(x) = x/|x|$ is the sign of $x$. Then, inserting (12) and (13) into (11) we obtain

$$\psi(x) = \frac{1}{8b} (\text{sign}(x - x_0 + b) - \text{sign}(x - x_0 - b)) + \frac{i}{4\pi b} \ln \frac{|x - x_0 + b|}{|x - x_0 - b|}$$  \hspace{1cm} (14)

We see that the function $\psi(x)$ in (14) consists of a local real part (sign) and a nonlocal imaginary part (log). For $t \neq 0$ it is sufficient to replace $x$ by $x - t$ in (8). Similar result is obtained for $\psi^*(x + t)$. As a result, the function $\Phi(x, t)$ is also nonlocal because it is the superposition of the two complex functions $\psi(x - t)$ and $\psi^*(x + t)$ in (8), which describe nonlocal objects moving with the speed of light in opposite directions. However, at $t = 0$ the imaginary parts cancel each other (see Fig. 1), and we recover our localized initial condition (8), because only the real parts of these functions, which are local, remain.

In all our figures time $t$ is measured in seconds (s), the coordinate $x$ is measured in "light seconds" (ls) and wave packet amplitudes are dimensionless. Fig. 2 corresponds to $t = 0.25 \text{ s}$. At this moment the real local parts of $\psi(x - t)$ and $\psi^*(x + t)$ have moved in opposite directions. The nonlocal imaginary parts of $\psi(x - t)$ and $\psi^*(x + t)$ have also shifted in opposite directions and no more cancel each other. At this time, the two waves overlap and we have

$$|\Phi(x, t)| \equiv |\psi(x - t) + \psi^*(x + t)| \neq |\psi(x - t)| + |\psi^*(x + t)|$$  \hspace{1cm} (15)
At $t = 1$ s in Fig. 3 the overlapping is small and we have

$$|\Phi(x,t)| \approx |\psi(x-t)| + |\psi^*(x+t)|$$

(16)

We see that the initial condition $\Phi(x,0)$ is local (Fig. 1) only because at $t = 0$ the nonlocal parts cancel each other completely by destructive interference. We may describe the appearance of nonlocality as a sort of “curtain effect”. The nonlocal nature of each wave packet $\psi(x-t)$ and $\psi^*(x+t)$ is hidden behind a “curtain” at the initial time and emerges immediately afterwards. Each of the nonlocal wave packets is complex and propagates at the speed of light.

In conclusion, we have illustrated Hegerfeldt’s theorem for classical wave packets. We see that the localization of wave packets corresponding to positive frequency is unstable and involves complex space structures.

Note that the localization of a positive frequency wave packet is not “complete”, because the time derivative of the function $\Phi(x,t)$ is nonlocal even at $t = 0$:

$$\left[ \frac{\partial \Phi(x,t)}{\partial t} \right]_{t=0} = \frac{i}{2\pi b} \left( \frac{1}{x-x_0-b} - \frac{1}{x-x_0+b} \right)$$

(17)

The wave equation being of second order demands two initial conditions: for the function itself and for its time derivative. The additional requirement of positivity of frequency replaces the second condition. There are no wave packets containing only positive frequency modes, which are localized together with their time derivative [7].

### 3 Relativistic quantum field

We turn now to relativistic quantum field theory. We show that the previous discussion is applicable to relativistic quantum particles. In this case the condition $\omega_k > 0$ appears naturally since the energy $E = \hbar\omega_k$ must be positive (we take $\hbar = 1$). We consider massless particles with no spin (“photons”). To simplify our consideration we use again
a 1+1-dimensional spacetime. In terms of second quantization we have the scalar field operator
\[
\hat{\psi}(x, t) = \int_{-\infty}^{+\infty} d\tilde{k} \left( a_k^\dagger e^{i(\omega_k t - kx)} + a_k e^{-i(\omega_k t - kx)} \right)
\]  
where \( d\tilde{k} = dk/(4\pi\omega_k) \) is a relativistic invariant measure and
\[
\omega_k = |k|
\]
with \( c = 1 \). The creation and annihilation operators \( a_k^\dagger \) and \( a_k \) of the photon with wave vector \( k \) obey the commutation relation
\[
\left[ a_k^\dagger, a_{k'} \right] = 4\pi\omega_k \delta(k - k')
\]
We construct a wave packet from a linear combination of normal modes.
\[
|\Phi_{x_0, b}(t)\rangle = \int_{-\infty}^{+\infty} d\tilde{k} \phi_{x_0, b}(k)e^{-i\omega_k t}a_k^\dagger|0\rangle
\]
Here \(|0\rangle\) is the vacuum state for the field \((18)\). The fact that our wave packet is obtained by the action of creation operators on the vacuum state implies that the state consists of normal modes with positive energy. As before, we chose the function \( \phi_{x_0, b}(k) \) so that the wave packet is localized at the time \( t = 0 \) in a domain with center \( x_0 \) and width \( 2b \),
\[
\phi_{x_0, b}(k) = (2\omega_k)^{1/2} \int_{-\infty}^{+\infty} dx \, e^{ikx}\Phi_{x_0, b}(x, 0)
\]
where
\[
\Phi_{x_0, b}(x, 0) = \frac{1}{(2b)^{1/2}} \Theta(b - |x - x_0|)
\]
The function \( \Phi_{x_0, b}(x, 0) \) is normalized to ensure the normalization of the state \(|\Phi_{x_0, b}(0)\rangle\) in \((21)\).

Let us introduce the operator \( \rho(x) \):
\[
\rho(x) = a^\dagger(x)a(x)
\]
where \( a^\dagger(x) \) and \( a(x) \) are defined by
\[
a^\dagger(x) = \int_{-\infty}^{+\infty} d\tilde{k}(2\omega_k)^{1/2} e^{-ikx}a_k^\dagger
\]
\[
a(x) = \int_{-\infty}^{+\infty} d\tilde{k}(2\omega_k)^{1/2} e^{ikx}a_k
\]
These operators satisfy the commutation relation

\[
[a(x), a^\dagger(x')] = \delta(x - x')
\]  

This construction follows the ideas of the construction of positions operators by Newton and Wigner [1]. We shall express the localization of our state \(|\Phi_{x_0,b}(t)\rangle\) in terms of the expectation value of the operator \(\rho(x)\). We call a state localized if the expectation value of \(\rho(x)\) in this state vanishes when \(x\) is outside a finite region. Our choice of \(\phi_{x_0,b}(k)\) in (22) and \(\Phi_{x_0,b}(x)\) in (23) guarantees that the state \(|\Phi_{x_0,b}(t)\rangle\) is localized at \(t = 0\) in the domain \([x_0 - b, x_0 + b]\), i.e.,

\[
\langle \Phi_{x_0,b}(0)|\rho(x)|\Phi_{x_0,b}(0)\rangle = \frac{1}{2b}\Theta(b - |x - x_0|)
\]  

Using (23) we obtain the time evolution of this quantity

\[
\langle \Phi_{x_0,b}(t)|\rho(x)|\Phi_{x_0,b}(t)\rangle = \int \int_0^{+\infty} d\tilde{k} d\tilde{k}' (4\omega_k \omega_{k'})^{1/2} e^{-i(k-k')x} \langle \Phi_{x_0,b}(t)|a_k^\dagger a_k|\Phi_{x_0,b}(t)\rangle
\]  

where \(\langle \Phi_{x_0,b}(t)|a_k^\dagger a_k|\Phi_{x_0,b}(t)\rangle\) is expressed using our form of the wave packet (21) as follows:

\[
\langle \Phi_{x_0,b}(t)|a_k^\dagger a_k|\Phi_{x_0,b}(t)\rangle = \int \int_0^{+\infty} dl dl' \phi_{x_0,b}(l)e^{i(\omega_l - \omega_l')t}(0)|a_l^\dagger a_l|0\rangle
\]  

Using the commutation relation (20) we integrate (29) over \(l\) and \(l'\) and then insert the result into (28). Taking into account the positivity of energy (19) and the form of the function \(\phi_{x_0,b}(k)\) in (22) we obtain

\[
\langle \Phi_{x_0,b}(t)|\rho(x)|\Phi_{x_0,b}(t)\rangle = \left| \int_{x_0-b}^{x_0+b} dx' \int_{-\infty}^{+\infty} dk e^{-ik|t| + ik(x-x')} \right|^2
\]  

By comparison with (7) we see that this quantity is equal to the absolute value squared of the classical function \(\Phi(x,t)\) up to the normalization constant. Our discussion of nonlocality remains, therefore, also valid in the quantum case, and the expression inside the absolute value in (30) is a superposition of two nonlocal wave packets that move in opposite directions at the speed of light. In the appendix give a second example using an analogy with Fermi’s problem [2].
Let us note that in quantum field theory localization depends on the observable. If a state is local from the point of view of one observable, it can be nonlocal from the point of view of another. In our example the expectation value of the operator $\rho(x)$ is local in the state $|\Phi_{x_0,b}(0)\rangle$. At the same time, the energy density of the field in the same state is nonlocal. Indeed, the energy density $T_{00}(x)$ of the free massless field (18) is

$$T_{00}(x) = \frac{1}{2} \left( \left( \frac{\partial \hat{\psi}}{\partial t} \right)^2 + \left( \frac{\partial \hat{\psi}}{\partial x} \right)^2 \right)$$

(31)

It contains the derivatives of the field operator. (As we have seen in classical case, the time derivative of the function $\Phi(x,t)$ is nonlocal even at $t = 0$). To determine the expectation value of $T_{00}(x)$ in the state $|\Phi_{x_0,b}(0)\rangle$ taking into account the positivity of energy (19) we first calculate this expectation value for a finite $t$ and then take the limit $t \to 0$. Using (18)-(23) obtain:

$$\langle \Phi_{x_0,b}(0)|T_{00}(x)|\Phi_{x_0,b}(0)\rangle = \frac{1}{4\pi b} \left( \frac{1}{|x - b|} + \frac{1}{|x + b|} - \frac{1 - \text{sign}(x - b) \text{sign}(x + b)}{\sqrt{|x - b|}\sqrt{|x + b|}} \right)$$

(32)

where we put $x_0 = 0$ to simplify the expression. This quantity is obviously nonlocal.

4 Conclusion

Positivity of energy for quantum fields (or frequency for classical fields) leads to a decomposition of localized wave packets in terms of nonlocal wave packets with long tails. The long tails, which cancel each other initially, appear immediately afterwards as the nonlocal wavepackets move in opposite directions. In our examples the long tails decay with the distance $x$ according to $b/x$ for $b/x \ll 1$, where $b$ is the size of the localized wave packet. They are precursors to the usual wave propagation. Although we may have instant interactions, these are not the result of superluminal propagation, but of “preformed” structures.

We shall study the interaction between nonlocal structures in a separate paper. We have then “contact interactions”, due to the overlapping of the long tails. We shall also
show that the photon clouds around atoms and molecules are nonlocal, which leads to
the precursor effect and eliminates the apparent deviation from causality in Fermi’s two-
atom problem. However, it is true that the two atoms “feel” each other instantaneously.
Even inside a relativistic theory (the wave equation is Lorenz invariant) there is place for
instantaneous interactions due to nonlocality.

Einstein’s relativistic events are associated to four dimensional points. Here we see
nonlocal but still relativistic events that are due to the instability of localization as shown
in the examples presented in this paper.

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APPENDIX

Here we show an analogy of our problem with Fermi’s two-atom problem. We prepare our
wave packet $|\Phi_{x_0,b}(t)\rangle$ “localized” at $t = 0$. At time $t$ we project this state on an second
wave packet $|\Phi_{x_1,b}(0)\rangle$, which is localized in a domain with center $x_1 \neq x_0$ and width $2b$,
and plays the role of a measurement device. We choose $x_1$ so that $x_1 - x_0 > 2b$. Then, at
$t = 0$ these two states do not overlap and the scalar product $\langle \Phi_{x_1,b}(0)|\Phi_{x_0,b}(t)\rangle$ vanishes.

We consider this scalar product as a function of $t$, i.e., at each moment $t$ we project the
evolving wave packet $|\Phi_{x_0,b}(x,t)\rangle$ on the localized state $|\Phi_{x_1,b}(0)\rangle$. As we have shown,
the initially localized packet, which evolves in time, is nonlocal immediately after $t = 0$
and our scalar product has a non-vanishing value. This can be interpreted as the second (localized) wave packet “feeling” the existence of the first one even at $t < x_1 - x_0 - 2b$ when the causal component of the first wave packet still did not reach the domain of localization of the second wave packet. The scalar product $\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle$ grows as the overlapping of the two wave packets increases (see Fig. 4). We expect some essential change of this growth when the main part of the first wave packet corresponding to the position of its local (“causal”) component reaches the domain of localization of the second wave packet. Then, as the moving component goes away, the scalar product decreases.

To show this, we write this scalar product using \eqref{psiphi1} in the following form

$$\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle = \int \int_{-\infty}^{+\infty} dk \phi^*_{x_1,b}(k) \phi_{x_0,b}(k') e^{-i\omega_k t} \langle 0 | a_k a_k^\dagger | 0 \rangle \quad (A1)$$

We perform the integration over $k'$ with the help of the commutation relation \eqref{comrel}. Then, inserting \eqref{comrel} and \eqref{psi1} we obtain

$$\langle \Phi_{x_1,b}(x,0) | \Phi_{x_0,b}(x,t) \rangle = \frac{1}{4\pi b} \int_{x_1-b}^{x_1+b} dx' \int_{x_0-b}^{x_0+b} dx'' \int_{-\infty}^{+\infty} dk e^{-i|k| t + ik(x'-x'')} \quad (A2)$$

Using a regularisation similar to \eqref{psib}, we integrate over $k$ and obtain

$$\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle = \frac{1}{4\pi ib} \int_{x_1-b}^{x_1+b} dx' \int_{x_0-b}^{x_0+b} dx'' \left( \frac{1}{t - x' + x'' - i0} - \frac{1}{t + x' - x'' - i0} \right) \quad (A3)$$

The integration over $x'$ and $x''$ and the rearrangement of terms give us

$$\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle = \psi_1(x_1 - x_0 + t - i0) - \psi_1(x_1 - x_0 - t + i0) \quad (A4)$$

where

$$\psi_1(x) = \frac{1}{4\pi ib} ((x - 2b) \ln(x - 2b) + (x + 2b) \ln(x + 2b) - 2x \ln(x)) \quad (A5)$$

Then, using \eqref{psiphi1}, \eqref{psib} we come to

$$\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle = \psi_2(x_1 - x_0 - t) + \psi^*_2(x_1 - x_0 + t) \quad (A6)$$

where

$$\psi_2(x) = \frac{1}{8b} (|x - 2b| + |x + 2b| - 2|x|)$$
\[
+ \frac{i}{4\pi b} (|x - 2b| \ln |x - 2b| + |x + 2b| \ln |x + 2b| - 2|x| \ln |x|)
\]

Fig. 5 shows the real part, the imaginary part and the absolute value of the scalar product \(\langle \Phi_{x_1,b}(0) | \Phi_{x_0,b}(t) \rangle\) as functions of \(t\) for two different values of the wave packet’s width \(b\). The real component is non-vanishing only in the time interval corresponding to the overlapping of the localized components. In contrast, the imaginary part is non-vanishing immediately after \(t = 0\), because it reflects the overlapping of nonlocal components. Fig. 5 also shows that the “causal” part of the effect is much bigger than the contribution of the long tails, if the size of the wave packet is much less than the distance between the domains of localization.
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b) $\mathcal{R}\langle \Phi_{2,\theta}(0)|\Phi_{0,\beta}(t)\rangle$

c) $\Im\langle \Phi_{2,\theta}(0)|\Phi_{0,\beta}(t)\rangle$

d) $\Im\langle \Phi_{2,\theta}(0)|\Phi_{0,\beta}(t)\rangle$

e) $|\langle \Phi_{2,\theta}(0)|\Phi_{0,\beta}(t)\rangle|$ 

f) $|\langle \Phi_{2,\theta}(0)|\Phi_{0,\beta}(t)\rangle|$