A Causal Alternative to Feynman’s Propagator

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The Feynman propagator used in the conventional in-out formalism in quantum field theory is not a causal propagator as wave packets are propagated virtually instantaneously outside the causal region of the initial state. We formulate a causal in-out formalism in quantum field theory by making use of the Wheeler propagator, the time ordered commutator propagator, which is manifestly causal. Only free scalar field theories and their first quantization are considered. We identify the real Klein Gordon field itself as the wave function of a neutral spinless relativistic particle. Furthermore, we derive a probability density for our relativistic wave packet using the inner product between states that live on a suitably defined Hilbert space of real quantum fields. We show that the time evolution of our probability density is governed by the Wheeler propagator, such that it behaves causally too.

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I. INTRODUCTION

Quantum field theory is a very successful theory. The Feynman rules are very simple to follow but stem from complicated underlying considerations. For example, in order to compute a certain transition amplitude, a particular Feynman diagram needs to be renormalized and computed before it can be related to observables (a cross section). The standard in-out formalism used to calculate Feynman diagrams has however two shortcomings:

• Transition amplitudes in the in-out formalism are not causal;

• Transition amplitudes in the in-out formalism are not real.
The standard in-out formalism is not causal in the following sense: the Feynman propagator that one uses to calculate diagrams in perturbation theory is not a causal propagator as it has non-vanishing support outside the past- and future light cone of a certain spacetime point $x$. In other words, the Feynman propagator $\Delta_F(x; x')$ does not vanish when $x$ and $x'$ are spacelike separated. This sense of causality is sometimes referred to as Einstein causality.

The standard in-out formalism is not real in the following sense: even for real scalar fields the quantum description is complex since creation operators only create the positive frequency part of a field and all negative frequency dependence is automatically projected out. Self-energies are therefore generically complex valued although we started the computation with real fields. In other words, the in-out effective action does not generate the correct quantum corrected equations of motion for the real scalar field.

Similar to unitarity, causality is an ingredient of fundamental importance of relativistic quantum field theories. Let us be very explicit about the following point: no one would claim that quantum field theory is not a causal theory. Expectation values can be expressed in terms of series of time ordered nested commutators (see e.g. [4, 5]), which makes them manifestly causal. We thus conclude that when calculating observables using Feynman propagators crucial cancellations must occur between various diagrams such that the final result is causal.

The approach which computes true expectation values without computing scattering amplitudes as an intermediate step is referred to as the in-in or Schwinger-Keldysh formalism [4, 6–10], for applications see [11–14]. The in-in formalism does not suffer from the shortcomings of the in-out formalism as mentioned above. Also, self-mass corrections to real propagators are purely real as they should. Hence, the interpretation of the self-mass corrections thus obtained is much more straightforward than in the in-out formalism.

The main idea that we outline in this paper is how to set up a real and causal first quantized description in perturbative quantum field theory in an in-out setting. We only develop the ingredients necessary to build a perturbative quantum field theory that meets these requirements, and we postpone the development of a perturbation theory itself to a future paper. Let us begin by recalling the first quantized picture in conventional quantum field theory before we explain where we differ from the standard approach. Quantum states in the conventional approach to quantum field theory are complex valued, just as in non-relativistic quantum mechanics. The reason is very

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1 Although the in-in formalism is perfectly causal, it is not manifest in all incarnations of the in-in formalism. The diagrammatic approaches of [15] and [16] are for instance not based on purely causal propagators.
simple to see in second quantization: a creation operator creates a positive frequency wave mode out of the vacuum \( \hat{a}_k^\dagger |0\rangle = |\omega_k, \vec{k}\rangle \), where \( \omega_k = (\vec{k}^2 + m^2)^{1/2} \) as usual. Now one can employ the superposition principle such that the positive frequency contribution \( \phi_+(x) \) to the real field \( \phi(x) \) is a quantum mechanical wave function:

\[
\Psi(x) = \phi_+(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \phi(\omega_k, \vec{k}) e^{-i\omega_k t + i\vec{k} \cdot \vec{x}}.
\]

Clearly, this wave function is complex valued. Furthermore, by making use of the inner product between fields that live on the Hilbert space of positive frequency solutions to the Klein Gordon equation one can straightforwardly find a probability density that, integrated over its domain of non-zero support, can be properly normalized to unity. See for example section 3.1 of [17] or section 14.2 of [18] where a similar interpretation is made. This probability density is the 0th component of the familiar Klein Gordon current given by:

\[
N^{KG}_0(x) = \phi_+^\dagger(x) i \partial_t \phi_+(x),
\]

The natural question that presents itself when writing down an equation like (1) and (2) is: why is \( \Psi(x) \) not the wave function in quantum field theory? In other words: why is \( \Psi(x) \) not the relativistic generalization of the wave function of ordinary quantum mechanics? The answer is that the candidate wave function \( \Psi(x) \) defined above does not behave causally (see e.g. [19, 20]). Advanced or retarded propagation of the candidate wave function \( \Psi(x) \) is governed by the Feynman propagator, which, as we emphasized before, is not a causal propagator. It is physically unacceptable to define a relativistic wave function that would virtually instantaneously spread outside the past and future light cone of its region of non-zero support. The Feynman propagator is however well suited to do perturbation theory as it is time ordered and hence a Green’s function (the solution to the Schrödinger equation is a time ordered evolution operator). Despite its obvious shortcomings, this is the reason that the Feynman propagator is so widely used when calculating Feynman diagrams.

We construct real quantum states \( |\phi\rangle \) that include both positive and negative frequency contributions \( \pm \omega_k \). Our wave function thus becomes the real field itself:

\[
\Psi(x) = \phi(x) = \phi_+(x) + \phi_-(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[ \phi(\omega_k, \vec{k}) e^{-i\omega_k t + i\vec{k} \cdot \vec{x}} + \phi(-\omega_k, \vec{k}) e^{+i\omega_k t + i\vec{k} \cdot \vec{x}} \right]. \tag{3}
\]

There is an additional problem concerning the localization of relativistic particles, i.e.: the standard Newton Wigner position operator suffers from non-locality problems that would prevent us from localizing a particle on scales smaller than its Compton wavelength. We will not address this problem here but present a solution in [21], which further complements a consistent first quantized interpretation of quantum field theory. Additionally, pair creation is often argued to fundamentally limit the localization of relativistic particles. This argument does not apply however since we are discussing real fields.
The positive definite inner product between real fields that includes positive and negative frequency solutions to the Klein Gordon equation \[22–24\] readily provides us with a positive definite probability density:

\[
J_0^P(x) = \frac{1}{2} \left[ \phi_+^*(x) i \hat{\partial}_t \phi_+(x) - \phi_-^*(x) i \hat{\partial}_t \phi_-(x) \right].
\] (4)

For real fields, one can easily check that the two currents (2) and (4) are equal.

What about the propagation of our quantum states, or of the probability density thus defined? Let us recall again that the Feynman propagator propagates complex valued wave functions in a manner that is not causal, but it is a Green’s function such that it can be used in perturbative quantum field theory. There exists, however, a propagator that meets all the necessary requirements: it is real, causal and it is a time ordered Green’s function such that we can use it in a perturbative expansion as well. This propagator is the time ordered commutator propagator, or Wheeler propagator. The Wheeler propagator is the real part of the Feynman propagator, or the average of the advanced and the retarded propagator. Only the Wheeler propagator propagates the entire real quantum field \(\phi(x)\) in a time ordered manner unlike the Feynman propagator. Ultimately, the idea is to formally set up a perturbation theory in quantum field theory using the Wheeler propagator instead of the Feynman propagator.

The structure of the paper is as follows. In section II we establish our notation and carefully develop a consistent first quantization in quantum field theory using real states. Also, we study various propagators to examine how they act on quantum states. In section III we consider how probabilities in our new setup of quantum field theory are defined. Finally, in section IV we discuss the role of the Wheeler propagator and see how it causally propagates probability densities. Throughout the paper we only consider free, real scalar field theories to keep the conceptual subtleties clear and postpone the discussion of interacting field theories to a future publication.

II. FIRST QUANTIZATION INCLUDING NEGATIVE FREQUENCY CONTRIBUTIONS

First quantization attempts to construct a relativistic quantum field theory for a single particle wave function with a probabilistic interpretation just as in non-relativistic quantum mechanics. Here, we do not consider second quantization, where creation and annihilation operators are introduced to conveniently describe multi-particle quantum states. The Lagrangian density for a real
The scalar field reads:

\[ L(\phi, \partial_\mu \phi) = -\frac{1}{2} \left( \eta^{\mu\nu} \partial_\mu \phi \partial_\nu \phi + \mu^2 \phi^2 \right), \]  

(5)

where we use the Minkowski metric \( \eta^{\mu\nu} = \text{diag}(-1, 1, 1, 1) \) and where \( \mu \) is the inverse of the reduced Compton wavelength:

\[ \mu = \frac{1}{\lambda_c} = \frac{mc}{\hbar}. \]  

(6)

The Klein Gordon equation of motion follows from equation (5) as usual as:

\[ (\Box - \frac{m^2 c^2}{\hbar^2}) \phi(x) = 0. \]  

(7)

Here, \( \Box \) is the d’Alembertian. Let us Fourier transform our field as usual as:

\[ \phi(x) = \int \frac{d^4k}{(2\pi)^4} \tilde{\phi}(k)e^{ikx}, \]  

(8)

where we employed the standard notation \( kx = \eta_{\mu\nu}k^\mu x^\nu \). Let us set \( \hbar = c = 1 \). When we substitute equation (8) in the Klein Gordon equation (7), we find the usual on shell condition \((k^0)^2 = \vec{k}^2 + m^2\), such that we can write:

\[ \tilde{\phi}(k) = 2\pi \delta(k^2 + m^2) \phi(k) e^{ikx}. \]  

(9)

We thus see that \( \tilde{\phi}(k) = 2\pi \delta(k^2 + m^2) \phi(k) \). We can clearly see that two separate contributions arise if we were to evaluate the delta function explicitly as we have on shell solutions with positive and negative frequency:

\[ \phi_{\pm}(x) = \int \frac{d^4k}{(2\pi)^4} \delta(k^2 + m^2) \theta(\pm k^0) \phi(k) e^{ikx} = \int \frac{d^3\vec{k}}{(2\pi)^3 2\omega_k} \phi(k_{\pm}) e^{\pm k \cdot x}, \]  

(10)

where \( \omega_k = (|\vec{k}|^2 + m^2)^{1/2} \) as usual and we defined the contravariant vector:

\[ k_{\pm} = (\pm \omega_k, \vec{k}). \]  

(11)

Throughout the paper we will refer to the \( \pm \) indices as positive and negative frequency indices. If one insists on keeping a manifestly Lorentz invariant expression, one can leave the delta function in equation (10) unevaluated. We thus have:

\[ \phi(x) = \phi_{+}(x) + \phi_{-}(x). \]  

(12)

Since we are studying real fields, we have \( \phi^*(\omega) = \phi(k) \) as usual, from which we conclude that \( \phi^*_{\pm}(x) = \phi_{\mp}(x) \).
A. Connecting the Schrödinger and Klein Gordon equations

Although the connection between Dirac’s equation and Schrödinger’s equation is obvious, one should appreciate that similar arguments apply to free scalar fields as well. In non-interacting scalar theories, one can factorize the Klein Gordon equation \( (7) \) as follows:

\[
\left( \frac{1}{c} \partial_0 + \sqrt{\mu^2 - \vec{\nabla}^2} \right) \left( \frac{1}{c} \partial_0 - \sqrt{\mu^2 - \vec{\nabla}^2} \right) \phi(x) = 0.
\]

The meaning of the square root of the derivative operator is defined in momentum space. In this equation and in the following few we reinstated \( \hbar \) and \( c \) explicitly again for clarity. Using equation \( (12) \) we thus see:

\[
\pm i \hbar \partial_0 \phi_{\pm}(x) = \pm mc^2 \sqrt{1 - \left( \frac{\hbar}{mc} \right)^2 \vec{\nabla}^2} \phi_{\pm}(x),
\]

These equations are sometimes called “spinless Salpeter” equations. In the non-relativistic limit where the relative spatial variations in the field are much smaller than the inverse Compton wavelength \( \vec{\nabla}^2 \phi_{\pm} \ll \left( \frac{mc}{\hbar} \right)^2 \) one obtains:

\[
\pm i \hbar \partial_0 \phi_{\pm}(x) = mc^2 \phi_{\pm} - \frac{\hbar^2}{2m} \vec{\nabla}^2 \phi_{\pm} - \frac{\hbar^4}{8m^3c^2} \vec{\nabla}^4 \phi_{\pm} - \ldots .
\]

Clearly, the positive and negative frequency parts of the Klein Gordon field satisfy a Schrödinger equation and its complex conjugate equation, respectively. We can thus make the following interpretation: The positive frequency and negative contributions to a quantum field are wave functions in the non-relativistic limit. Please note that these considerations only apply to free theories.

In the literature one can sometimes read confusing statements that the negative frequency contributions have negative energy\(^3\). The reason for these statements is that the “Hamiltonian” appearing in Schrödinger’s equation is indeed negative for negative frequency modes. The appropriate Hamiltonian to consider, however, is the Klein Gordon Hamiltonian, which is as usual given by:

\[
H = \int d^4x \partial_0 T^{00} = \frac{1}{2} \int d^3\vec{x} \left( (\partial_0 \phi)^2 + \vec{\nabla} \phi \cdot \vec{\nabla} \phi + m^2 \phi^2 \right)
\]

\[
= \frac{1}{2} \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2) \left| k^0 \right| \left| \phi(k) \right|^2 .
\]

\(^3\) These “negative energy” contributions were considered problematic in the early days of quantum field theory and led Dirac to develop his picture of an infinite sea of occupied fermionic states which has now become obsolete.
We thus conclude that negative frequency modes have positive energy as they should\(^4\). This point is of course well known in the literature, but we think it is important to mention it explicitly.

As \(\phi_+(x)\) satisfies a Schrödinger equation in the non-relativistic regime and because it has positive energies, it was argued some decades ago that \(\phi_+(x)\) perhaps was a promising candidate for the relativistic wave function\(^5\). It was realized however, that these “wave functions” would not spread in a causal manner\([19,20]\). We take the following point of view:

- The entire field \(\phi(x)\) and not just its positive frequency part \(\phi_+(x)\) is a wave function in relativistic quantum field theory. The dynamics of the wave function \(\phi(x)\) is governed by the Klein Gordon equation;

- The probability density follows from the definition of the inner product on the positive and negative Hilbert spaces.

In other words: we include the negative frequency contributions to a quantum field in what we define to be the wave functions in quantum field theory. Note that \(\hbar\) explicitly appears in the Klein Gordon equation\([7]\), as is well known, so we can indeed interpret it as a quantum equation that governs the time evolution of the real wave function \(\phi(x)\). In the next sections, we properly define quantum states, study how they are propagated by various propagators and finally, we associate probabilities to the inner product of a quantum state with itself and study how this probability density is propagated in time.

### B. Quantum States in Quantum Field Theory

Let us firstly recall how wave packets are constructed in the conventional approach to quantum field theory. Here, the crucial point is that a quantum state is derived from the positive frequency contribution to a quantum field only. Those states are therefore complex valued. For example, equation (4.65) of Peskin and Schroeder\([33]\) reads:

\[
|\psi_{\text{PS}}\rangle = \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{\sqrt{2} \omega_k}{\sqrt{2}\omega_k} \phi(\vec{k}) |\vec{k}\rangle ,
\]

\(^\text{\(4\)}\) We would like to emphasize that we do not introduce fields with negative energy, contrary to the approaches taken in e.g.\([25,26]\). We merely include the Hilbert space of negative frequency solutions to the Klein Gordon equation into our description of quantum field theory such that the real field itself can be interpreted as a quantum mechanical wave function.

\(^\text{\(5\)}\) This is one way to view the Feynman-Stückelberg interpretation of quantum field theory\([30,31]\).
where the subscript “PS” refers to Peskin and Schroeder. In order to better illustrate the point we would like to make, we modify this equation slightly to:

\[
|\phi_{PS}\rangle \rightarrow \int \frac{d^3 \vec{k}}{(2\pi)^3 2\omega_k} \phi(\omega_k, \vec{k}) |\omega_k, \vec{k}\rangle. 
\]  

(18)

Equation (17) and (18) differ in two respects: normalization and a notational difference as we explicitly include the \(k^0\) dependence. Unlike Peskin and Schroeder, we insist on a Lorentz invariant definition for the states. One can express any state in a manifestly Lorentz invariant way as:

\[
|\tilde{\phi}\rangle = \int d(LIPS) \tilde{\phi}(k^0, \vec{k}) |k^0, \vec{k}\rangle,
\]  

(19)

where the Lorentz invariant phase space (LIPS) element for one particle is in the standard approach to quantum field theory given by:

\[
d(LIPS) = \frac{d^4 k}{(2\pi)^3} \delta(k^2 + m^2) \theta(k^0) \frac{d^3 \vec{k}}{2\omega_k} \delta(k^0 - \omega_k).
\]  

(20)

It is clear from equations (18) and (20) above that in the Peskin and Schroeder state (17) only positive frequencies \(+\omega_k\) contribute:

\[
|\phi_{PS}\rangle = |\phi_+\rangle,
\]  

(21)

where we added a + sign to the right hand side of this equation to make this explicit.

Now let us discuss how we define quantum states in our new setup of quantum field theory. Given the fact that we can interpret a real scalar field as a wave function in relativistic quantum mechanics, we can define a Lorentz invariant state for our field as follows:

\[
|\phi\rangle = \int \frac{d^4 k}{(2\pi)^3} \delta(k^2 + m^2) \phi(k) |k\rangle
\]  

(22a)

\[
\langle \phi | = \int \frac{d^4 k}{(2\pi)^3} \delta(k^2 + m^2) \phi^*(k) \langle k |.
\]  

(22b)

Clearly, a quantum state is a superposition of various wave modes \(|k\rangle\) with a certain amplitude \(\phi(k)\) as usual. If one evaluates the delta function the positive and negative frequency modes appear again such that the state of a field is a superposition of positive and negative frequency states:

\[
|\phi\rangle = |\phi_+\rangle + |\phi_-\rangle,
\]  

(23)

---

6 The Lorentz invariant normalization of quantum states appears for example in [34] formula 3.4.2.

7 See for instance Ryder’s formula (4.4) [49].

8 The exclusion of negative frequency states is essentially due to Feynman and Stückelberg [30–32] who understood negative frequency states as Hermitian conjugate positive frequency states in the context of charged fields.
where:
\[
|\phi_\pm\rangle = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2)\theta(\pm k^0)\phi(k)|k\rangle = \int \frac{d^3\vec{k}}{(2\pi)^3 2\omega_k} \phi(k_\pm)|k_\pm\rangle,
\]
and where:
\[
|k_\pm\rangle = |\pm \omega_k, \vec{k}\rangle.
\]

It is of fundamental importance to realize that, unlike the conventional approach taken in the quantum field theoretical literature as in equation (17), our quantum state (22) includes the negative frequency contributions. This makes our quantum state real.

The inner product between momentum basis bras and state kets is naturally obtained by demanding that:
\[
\langle k_\pm|\phi\rangle = \phi_\pm(k),
\]
such that:
\[
\langle k_\alpha|k'_\beta\rangle = (2\pi)^3 2\omega_k \delta^{(3)}(\vec{k} - \vec{k}')\delta_{ab},
\]
where \(a\) and \(b\) are the frequency indices \(\pm\). This relation was first introduced by Hennaux and Teitelboim, who presented a worldline discussion of the supersymmetric particle [22]. We can now introduce spacetime kets as the covariant on shell Fourier transform of the momentum kets:
\[
|\vec{x}\rangle = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2)e^{-ik\vec{x}}|k\rangle = |x_+\rangle + |x_-\rangle,
\]
where:
\[
|x_\pm\rangle = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2)\theta(\pm k^0)e^{-ik\vec{x}}|k_\pm\rangle = \int \frac{d^3\vec{k}}{(2\pi)^3 2\omega_k} e^{-ik\pm \vec{x}}|k_\pm\rangle,
\]
\[
\langle x_\pm| = \int \frac{d^3\vec{k}}{(2\pi)^3 2\omega_k} e^{ik\pm \vec{x}}\langle k_\pm|.\]

The sign in both exponents is chosen to give the standard sign for the Fourier transform in equation (8) as we show below in equation (35). Equation (28) merits another remark. If we compare this equation for \(|\vec{x}\rangle\) with equation (22a) for \(|\phi\rangle\), we can identify \(\phi(k) \leftrightarrow e^{-ik\vec{x}}\). In other words: the state \(|\vec{x}\rangle\) corresponds to a superposition of plane wave modes, i.e.: a non-normalizable “wavepacket” of plane waves. The inverse Fourier relations are given by:
\[
|k_\pm\rangle = \pm \int d^3\vec{x} e^{ik\pm \vec{x}} i\partial_0|x_\pm\rangle,
\]
\[
\langle k_\pm| = \pm \int d^3\vec{x} e^{-ik\pm \vec{x}} i\partial_0\langle x_\pm|.\]
Here, we defined a time derivative that acts in the following way on two test functions $f(x)$ and $g(x)$:

$$ f(x) \partial_0 g(x) = f(x)\partial_0 g(x) - g(x)\partial_0 f(x). $$  

(31)

Having carefully defined the spacetime states, we find:

$$ \phi(x) = \phi_+(x) + \phi_-(x) = \langle x_+ | \phi \rangle + \langle x_- | \phi \rangle = \langle x | \phi \rangle. $$  

(32)

We can furthermore derive:

$$ |\phi_\pm\rangle = \mp \int d^3 \vec{x} \phi_\pm(x) i \partial_0 |x_\pm\rangle. $$  

(33)

Using (29) and the positive definite momentum space inner product (27) one easily derives:

$$ \langle x_\pm | k_\pm \rangle = e^{ik_\pm x} $$  

(34a)

$$ \langle k_\pm | x_\pm \rangle = e^{-ik_\pm x} $$  

(34b)

$$ \langle x_\pm | k_\mp \rangle = 0 $$  

(34c)

$$ \langle k_\pm | x_\mp \rangle = 0. $$  

(34d)

### C. Inner Products and the Identity Operator

We can also compute various position space inner products. The inner product between the positive and negative frequency modes separately yields the two Wightman functions:

$$ \Delta^\pm(x-x') = \pm i \langle x_\pm | x_\mp' \rangle = \pm i \int \frac{d^4k}{(2\pi)^3} \delta(k^2+m^2)\theta(\pm k^0)e^{ik(x-x')} = \pm i \int \frac{d^3k}{(2\pi)^3}2\omega_k e^{ik_\pm(x-x')}.$$  

(35)

The $\pm i$ in the definition of the Wightman functions becomes apparent later when we discuss propagators. Moreover, it is important to stress that our $\pm$ frequency indices are very different from the Schwinger-Keldysh indices often used in the in-in formalism in out-of-equilibrium quantum field theory. We also find:

$$ \langle x_\pm | x_\mp' \rangle = 0. $$  

(36)

The Wightman functions furthermore obey:

$$ \Delta^+(x-x') = -\Delta^-(x'-x) $$  

(37a)

$$ [\Delta^\pm(x-x')]^* = \Delta^\mp(x-x'). $$  

(37b)
The positive definite inner product between two arbitrary states follows from equation (22) as:

\[ \langle \chi | \phi \rangle = \int \frac{d^4 k}{(2\pi)^3} \delta(k^2 + m^2) \chi^*(k) \phi(k) = \int \frac{d^3 k}{(2\pi)^3 2\omega_k} \left[ \langle \chi | k_+ \rangle \langle k_+ | \phi \rangle + \langle \chi | k_- \rangle \langle k_- | \phi \rangle \right] \] (38)

which we can easily verify by for example applying it to \(|k_\pm]\rangle\). To derive the position space identity operator let us consider objects like \(\langle x_\pm | x'_\pm \rangle\) derived in equation (35). Inserting the following operator leaves these functions unchanged:

\[ \hat{I}_\pm = \pm \int d^3 \vec{x} |x_\pm\rangle i \overset{\leftrightarrow}{\partial_0} \langle x_\pm|, \] (41)

such that the position space identity operator on the total space of solutions is given by:

\[ \hat{I} = \int d^3 \vec{x} |x_+\rangle i \overset{\leftrightarrow}{\partial_0} \langle x_+| - |x_-\rangle i \overset{\leftrightarrow}{\partial_0} \langle x_-|. \] (42)

D. Propagators, Propagation Laws and Composition Laws

In this subsection, we derive various propagators for our quantum field. Intuitively, it is important to realize that propagators only propagate a state but do not contain information about the state itself. In other words: the wave mode \(|k\rangle\) of a certain state has an amplitude \(\phi(k)\) as in equation (22a). Wave packets can thus be constructed by the principle of superposition. Propagators do not contain any of this information. The amplitude of a certain wave mode \(|k\rangle\) for a propagator is just the plane wave \(\phi(k) = e^{-ikx}\). A propagation law captures how a propagator acts on a certain wave function, whereas a composition law captures how a propagator acts on another propagator.

1. Wightman propagators

We have already encountered the two Wightman functions in equation (35), given by:

\[ \Delta^\pm(x - x') = \pm i \langle x_\pm | x'_\pm \rangle. \] What we discuss here is how they act on the wave functions. By making
use of our identity operator \((41)\) one can straightforwardly show that:

\[
\phi_\pm(x) = \pm i \int d^3\vec{x}' \langle x_\pm | x_\pm' \rangle \partial_{t'} \phi_\pm(x') = \int d^3\vec{x}' \Delta_\pm(x - x') \partial_{t'} \phi_\pm(x') .
\] (43)

The propagators for positive and negative frequency wave functions are the positive and negative frequency Wightman propagators, respectively. Clearly, a wave function at a time \(t'\) is transformed to a wave function at another time \(t\), where at the moment \(t\) can be either earlier or later than \(t'\). It is important to realize that information about the state, i.e.: the specific superposition of wave modes in \((22)\), is always contained in \(\phi_\pm\), whereas the propagation of a state is governed by the Wightman functions. Wightman propagators can also act on the complex conjugate wave functions:

\[
\phi_\mp^*(x) = \pm i \int d^3\vec{x}' \phi_\mp^*(x') \partial_{t'} \phi_\pm(x') \leftrightarrow \partial_{t'} \frac{\delta}{\delta \phi_\pm(x')} = \int d^3\vec{x}' \phi_\mp^*(x') \partial_{t'} \Delta_\pm(x' - x) .
\] (44)

Here, we have made use of equation \((35)\). Moreover, we can easily see that:

\[
\int d^3\vec{x}' \Delta_\pm(x - x') \partial_{t'} \phi_\mp(x') = 0
\] (45)

The Wightman propagators satisfy the following composition laws:

\[
\int d^3\vec{x}'' \Delta_\pm(x - x'') \partial_{t''} \Delta_\pm(x'' - x') = \Delta_\pm(x - x') ,
\] (46)

which we prove straightforwardly by making use of the integral representation \((35)\). It will come as no surprise that the mixed composition laws for the Wightman propagators vanish:

\[
\int d^3\vec{x}'' \Delta_\pm(x - x'') \partial_{t''} \Delta_\bar{\pm}(x'' - x') = 0 .
\] (47)

2. Feynman propagator

The Feynman propagator ensures that the “right to left” direction of propagation in equation \((43)\) coincides with the direction of increasing time:

\[
\theta(t - t') \phi_\pm(x) = \int d^3\vec{x}' \Delta_F(x - x') \partial_{t'} \phi_\pm(x')
\] (48a)

\[
\theta(t' - t) \phi_\mp^*(x) = \int d^3\vec{x}' \phi_\mp^*(x') \partial_{t'} \Delta_F(x - x') ,
\] (48b)

where the Feynman propagator is the time ordered positive frequency Wightman propagator:

\[
\Delta_F(x - x') = iT[(x_+ | x_+')] = i\theta(t - t') \langle x_+ | x_+' \rangle + i\theta(t' - t) \langle x_+ | x_+' \rangle
\] (49)

\[
= i \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2) \theta(k^0)T \left[ e^{ik(x-x')} \right] .
\]
Here, $T$ denotes the time ordering symbol. This form shows explicitly that the Feynman propagator describes the on shell time ordered propagation of the positive frequency modes of a field. In other words, the Feynman propagator is a retarded propagator for positive frequency modes. Also, we see that the Feynman propagator is an advanced propagator for the complex conjugates of positive frequency modes. Since we know that $\phi^*_+(x) = \phi_-(x)$, we conclude from equation (48b) that the Feynman propagator is an advanced propagator of the negative frequency contributions too. We can bring equation (49) in the conventional form by also Fourier transforming the Heaviside step functions:

$$\Delta_F(x-x') = i \int \frac{dE}{2\pi} \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[ \frac{1}{E + i\epsilon} e^{-iE(t-t') + ik_+(x-x')} - \frac{1}{E - i\epsilon} e^{-iE(t-t') - ik_+(x-x')} \right]$$

$$= \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2 - i\epsilon} e^{ik(x-x')} ,$$

(50)

where we shifted the $E$ integration appropriately in the second line. Alternatively, we can rewrite the equation above as:

$$\Delta_F(x-x') = P \left[ \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2} e^{ik(x-x')} \right] + i\pi \int \frac{d^4k}{(2\pi)^4} \delta(k^2 + m^2) e^{ik(x-x')} ,$$

(51)

where we have made use of the Sokhotski-Plemelj or Sokhotsky-Weierstrass formula, also known as Dirac’s rule:

$$\frac{1}{\mu \pm i\epsilon} = P \frac{1}{\mu} \mp i\pi\delta(\mu) ,$$

(52)

where $P$ denotes the Cauchy principal value. The anti-Feynman or anti-time ordered propagator ($\overline{T}$) is now given by:

$$\Delta_{AF}(x-x') = i\overline{T}[(x_+|x'_+)] = i\theta(t' - t)(x_+|x'_+) + i\theta(t - t')(x'_+|x_+)$$

$$= \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2 + i\epsilon} e^{ik(x-x')} .$$

(53)

Let us now discuss the various composition laws for the Feynman propagator. Firstly, a Feynman propagator can act on another Feynman propagator:

$$\int d^3x'' \Delta_F(x-x'') \partial_\nu \Delta_F(x''-x') = \theta(t-t'')\theta(t''-t')\Delta^+(x-x') + \theta(t''-t)\theta(t'-t'')\Delta^-(x-x') ,$$

(54)

where it is crucially important to make use of the integral representation of the Feynman propagator in equation (51) in order to take the distributional character of the propagator properly into account. If we time order the expression above, i.e.: we require the latest to the left convention,
we find the composition law for the Feynman propagator:

\[
T \left[ \int d^3 \vec{x}'' \Delta_F(x - x'') \frac{\partial}{\partial t'} \Delta_F(x'' - x') \right] = \theta(t - t') \int d^3 \vec{x}'' \Delta_F(x - x'') \frac{\partial}{\partial t'} \Delta_F(x'' - x') + \theta(t' - t) \int d^3 \vec{x}'' \Delta_F(x' - x'') \frac{\partial}{\partial t''} \Delta_F(x'' - x) = \Delta_F(x - x') \left|_{t'' \neq t} \right. + \frac{1}{2} \Delta_F(x - x') \left|_{t'' = t} \right.
\]

Also, we can study how a Feynman propagator or anti-Feynman propagator acts on our Wightman functions. By making use of equation (50) and of several complex contour integrations one can show:

\[
\int d^3 \vec{x}'' \Delta_F(x - x'') \frac{\partial}{\partial t'} \Delta^{\pm} (x'' - x') = \pm \theta(\mp t \mp t'') \Delta^{\pm} (x - x'),
\]

\[
\int d^3 \vec{x}'' \Delta_{AF}(x - x'') \frac{\partial}{\partial t'} \Delta^{\pm} (x'' - x') = \mp \theta(\mp t \mp t'') \Delta^{\pm} (x - x').
\]

Apart from being a propagator, the Feynman propagator is also a Green’s function for the Klein Gordon equation. By making use of equation (50) one can verify that:

\[
(-\partial^2 + m^2) \Delta_F(x - x') = \delta^{(4)}(x - x'),
\]

such that the solution of \((-\partial^2 + m^2) \phi_+(x) = \tilde{J}(x)\) is:

\[
\phi_+(x) = \tilde{\phi}^0(x) + \int d^4 x' \Delta_F(x - x') \tilde{J}(x').
\]

Here, \(\tilde{\phi}^0(x)\) is a complex valued solution to the homogeneous Klein Gordon equation, and \(\tilde{J}\) is a complex valued source. Note that the Feynman propagator is complex valued and is therefore certainly not the Green’s function of the real scalar field \(\phi\). It can however be the Green’s function of e.g. the positive frequency contribution to our real field.

3. Commutator Propagator

So far, we have introduced the two Wightman and Feynman propagators. The former propagate the positive and negative frequency contributions to a real field, whereas the latter act as retarded and advanced propagators for these contributions, respectively. There is, however, another propagator worth discussing. It is the commutator propagator and it propagates the entire field, i.e. both its positive and negative frequency contributions:

\[
\phi(x) = \int d^3 \vec{x}' \Delta_C(x - x') \frac{\partial}{\partial t'} \phi(x')
\]
where the commutator propagator \( \Delta_C(x - x') \) is given by:

\[
\Delta_C(x - x') = i\eta^{ab} \langle x_a | x' b \rangle - i \langle x_+ | x'_- \rangle = \Delta^+(x - x') + \Delta^-(x - x').
\] (60)

Its integral representation reads:

\[
\Delta_C(x - x') = i \int \frac{d^4k}{(2\pi)^3} \delta(k^2 + m^2) \epsilon(k^0) e^{ik(x - x')},
\] (61)

where \( \epsilon(k^0) \) is sign function as before. It is important to realize that the commutator propagator satisfies the following relations:

\[
\Delta_C(x - x') \big|_{t = t'} = 0 \quad (62a)
\]

\[
\partial_t \Delta_C(x - x') \big|_{t = t'} = \delta^3(\vec{x} - \vec{x}'). \quad (62b)
\]

These identities are important for the following reason:

\[
\lim_{t \to t'} \phi(x) = \int d^3\vec{x}' \Delta_C(x - x') \partial_t \phi(x') \big|_{t = t'} - \int d^3\vec{x}' \phi(x') \partial_t \Delta_C(x - x') \big|_{t = t'}
\]

\[
= \phi(\vec{x}, t').
\] (63)

Thus at time coincidence no propagation of the field has occurred. The commutator propagator satisfies the following composition law:

\[
\Delta_C(x - x') = \int d^3\vec{x}'' \Delta_C(x - x'') \partial_{t''} \Delta_C(x'' - x').
\] (64)

4. Wheeler Propagator

Clearly, the commutator propagator is not a Green’s function as it does not satisfy the inhomogeneous Klein Gordon equation. Let us therefore define the Wheeler propagator as the time ordered commutator propagator:

\[
\Delta_W(x - x') = \frac{1}{2} T[\Delta_C(x - x')] = \frac{\epsilon(t - t')}{2} \Delta_C(x - x').
\] (65)

The last identity follows from the anti-symmetry of the commutator. The Wheeler propagator is thus symmetric in its arguments\(^9\). We follow \(^37\) in calling the time ordered commutator the Wheeler propagator\(^10\) as it appears implicitly in Wheeler and Feynman’s absorber theory\(^38\).

Wheeler’s two point function is also the average of the advanced and retarded propagator\(^39\, 40\):

\[
\Delta_W(x - x') = \frac{1}{2} \left( \Delta_A(x - x') + \Delta_R(x - x') \right),
\] (66)

\(^9\) This propagator appears in a classical context in \(^35\, 36\).

\(^{10}\) We do not agree however with the statement made in \(^37\) that the Wheeler propagator lacks on shell propagation, as is clear from equation \(^69\).
Moreover, the Wheeler propagator satisfies the following propagation law:

\[
\Delta_R(x - x') = \theta(t-t')\Delta_C(x - x') \quad (67a)
\]
\[
\Delta_A(x - x') = -\theta(t'-t)\Delta_C(x - x'). \quad (67b)
\]

Moreover, the Wheeler propagator satisfies the following propagation law:

\[
\frac{\epsilon(t-t')}{2}\phi(x) = \int d^3x'\Delta_W(x - x')\partial_{x'}\phi(x'). \quad (68)
\]

Hence, like the commutator propagator, the Wheeler propagator propagates the entire real quantum field. Note that this is natural since Wheeler’s two point function is real unlike the Feynman propagator. The Wheeler propagator has the following integral representations:

\[
\Delta_W(x - x') = \frac{i}{2} \int \frac{d^4k}{(2\pi)^4} \delta(k^2 + m^2)\epsilon(k^0)T \left[ e^{ik(x-x')} \right]
\]
\[
= \frac{i}{2} \int \frac{d^4k}{(2\pi)^4} \delta(k^2 + m^2)\epsilon(k^0)\epsilon(t-t')e^{ik(x-x')}
\]
\[
= \frac{1}{2} \int \frac{d^4k}{(2\pi)^4} \left[ \frac{1}{k^2 + m^2 + i\epsilon} + \frac{1}{k^2 + m^2 - i\epsilon} \right] e^{ik(x-x')} \quad (69)
\]

where on the second line we used the Fourier representation of the Heaviside step function. The Wheeler propagator is thus given by the real part of the Feynman propagator:

\[
\Delta_W(x - x') = \frac{1}{2} \left( \Delta_F(x - x') + \Delta_{AF}(x - x') \right) = \Re \left[ \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2} e^{ik(x-x')} \right]
\]
\[
= \Re \Delta_F(x - x'). \quad (70)
\]

Here, we used Dirac’s rule in equation [52] again. Clearly, this would equally well allow us to refer to the Wheeler propagator as the “principal part propagator”, see for instance [41]. Let us now discuss the composition law for the Wheeler propagator. A Wheeler propagator acts on another Wheeler propagator as follows:

\[
\int d^3x''\Delta_W(x - x'')\partial_{x''}\Delta_W(x'' - x') = \frac{1}{4}\Delta_C(x - x')\epsilon(t-t'')\epsilon(t'' - t'). \quad (71)
\]

Here, we made frequent use of equation [60]. Like the composition law of the Feynman propagator, we should time order the expression above. We thus derive:

\[
T \left[ \int d^3x''\Delta_W(x - x'')\partial_{x''}\Delta_W(x'' - x') \right] = \frac{1}{2}\Delta_W(x - x')\epsilon(t-t'')\epsilon(t'' - t'). \quad (72)
\]

We can recognize this equation as a composition law if we require \( t < t'' < t' \cup t' < t'' < t \):

\[
\Delta_W(x - x') = 2T \left[ \int d^3x''\Delta_W(x - x'')\partial_{x''}\Delta_W(x'' - x') \right]_{t < t'' < t'} \cup t' < t'' < t. \quad (73)
\]
The Wheeler propagator is not only a propagator, it is also a Green’s function of the Klein Gordon equation because of the time ordering. One can again easily see that:

\[ (-\partial^2 + m^2)\Delta_W(x - x') = \delta^{(4)}(x - x'), \]  

(74)

where we have made use of equation (69). The solution of \((-\partial^2 + m^2)\phi(x) = J(x)\) is thus:

\[ \phi(x) = \phi^0(x) + \int d^4x' \Delta_W(x - x')J(x'). \]  

(75)

Here, \(\phi^0(x)\) is a real solution to the homogeneous Klein Gordon equation. Finally, note that the Wheeler propagator is the Green’s function of the real scalar field \(\phi\), and not just of the complex valued positive frequency contribution \(\phi_+\) as the Feynman propagator is.

### III. PROBABILITY DENSITIES IN QUANTUM FIELD THEORY

Given our wave function interpretation of the real quantum field \(\phi\) as presented above, it is natural to define probability densities analogous to quantum mechanics. In quantum mechanics, the absolute value squared of a quantum mechanical wave function represents a probability distribution function of a single quantum mechanical particle, whose dynamics is governed by Schrödinger’s equation. The absolute value squared of a quantum mechanical wave function can be used as a probability measure because firstly it is positive and, secondly, it can be normalized to unity when integrated over its domain. The natural candidate for a probability density in relativistic quantum mechanics stems from the inner product between a quantum state with itself as we show shortly. The probability densities thus obtained are positive and can be normalized to unity too.

In the conventional approach to quantum field theory this natural generalization of quantum mechanics is problematic as only the positive frequency modes are included in wave packets and the negative frequency modes do not contribute. The propagation of these wave packets is, as we have seen above, governed by the Feynman propagator. The wave packets therefore spread non-causally. We solve this problem by properly including the negative frequency contributions in the wave packets such that their propagation is mediated by Wheeler’s propagator. We therefore have a normalized probability density at our disposal that spreads in a causal manner. This allows us to build a consistent first quantized picture in quantum field theory that naturally generalizes quantum mechanics to a relativistic setting.
A. A Normalized Probability Density and the Hadamard Propagator

In our setup of quantum field theory we require:

\[ \frac{1}{2} \langle \phi | \phi \rangle \equiv 1. \]  

(76)

Inserting the identity operator from equation (42) yields:

\[ 1 = 1 = \frac{1}{2} \int d^3 \vec{x} \langle \phi | x_+ \rangle \partial_0 \phi_+ - \langle \phi | x_- \rangle \partial_0 \phi_- \]  

(77)

\[ = \frac{1}{2} \int \frac{d^3 \vec{k}}{(2\pi)^3 2\omega_k} \left[ |\phi(k_+)|^2 + |\phi(k_-)|^2 \right] \]

\[ = \frac{1}{2} \int \frac{d^4 \vec{k}}{(2\pi)^4 \delta(k^2 + m^2)} |\phi(k)|^2. \]

The momentum space realization of this inner product is discussed for example in [42] where the author considers a stochastic interpretation of the fields. Halliwell and Ortiz discuss in [23] both the position space and momentum space realization in the context of the sum over histories interpretation of quantum field theory. Their work was inspired by earlier work of Henneaux and Teitelboim [22]. In a slightly different form the inner product can also be found in [24], also see [43]. The factor of 1/2 that appears in (77) is motivated by the canonical form of the Hamiltonian in equation (16). It is clear from equation (77) that plane waves cannot be normalized. One really needs a wave packet, i.e.: a superposition of various wave modes with a certain amplitude, such that the integrals in (77) converge. Note that a single plane wave does not meet this requirement and is therefore not a suitable wave packet. We can thus identify a probability current:

\[ J^P_\mu(x) = \frac{1}{2} \left[ \phi_+(x) \partial_\mu \phi_+ - \phi_-(x) \partial_\mu \phi_- \right], \]

(78)

which is conserved for free theories in the usual sense:

\[ \partial^\mu J^P_\mu(x) = 0, \]

(79)

where we have used the Klein Gordon equation. We identify the 0th component of the probability current as the probability density, given a wave function \( \phi(x) \):

\[ \rho_P(x) = J^P_0(x) = \frac{1}{2} \left[ \phi_+(x) \partial_t \phi_+ - \phi_-(x) \partial_t \phi_- \right]. \]

(80)

From the third line in equation (77) one can clearly see that the probability density is both real and positive. Given a spacelike region \( \mathcal{A} \), the probability of finding a particle in this region for
some observer thus follows as:

\[ P = \int_{\mathcal{A}} d^3 \vec{x} J_0^P(x) = \int_{\mathcal{A}} d^3 \vec{x} \rho_P(x) = \frac{1}{2} \int_{\mathcal{A}} d^3 \vec{x} \left[ \phi_+^*(x)i \partial_t \phi_+(x) - \phi_-^*(x)i \partial_t \phi_-(x) \right]. \]  

We already tentatively used the word particle in defining the probability above. We make this statement more precise shortly. Let us however first define the statistical propagator, or Hadamard propagator as:

\[ \Delta_H(x-x') = i \Delta^+(x-x') - i \Delta^-(x-x') = -\langle x_+ | x'_+ \rangle - \langle x_- | x'_- \rangle \]

\[ = -\int \frac{d^4 k}{(2\pi)^3} \delta(k^2 + m^2) e^{ik(x-x')} = -\int \frac{d^3 \vec{k}}{(2\pi)^3 2\omega_k} \left[ e^{i k_+(x-x')} + e^{i k_-(x-x')} \right]. \]  

We can straightforwardly relate the Hamadard propagator to the imaginary part of the Feynman propagator:

\[ \Delta_H(x-x') = -2\Im \Delta_F(x-x'). \]

The Hadamard propagator satisfies the following composition law in terms of the commutator propagator:

\[ \int d^3 \vec{x}' \Delta_C(x-x'') \partial_{x'} \Delta_H(x''-x') = \Delta_H(x-x'). \]

The reason for introducing the Hadamard propagator now becomes apparent. We can now show that:

\[ \frac{1}{2} \langle \phi | \phi \rangle = \frac{1}{2} \int d^3 \vec{x} d^3 \vec{x}' \phi(x) \partial_{x'} \Delta_H(x-x') \partial_{x'} \phi(x') \bigg|_{t=t'} = 1. \]

This inner product can also be found in \cite{23}. The Hadamard propagator thus offers an alternative way of evaluating the probability for finding a particle in our spacelike region \( \mathcal{A} \) for a particular observer:

\[ P = \frac{1}{2} \int_{\mathcal{A}} d^3 \vec{x} d^3 \vec{x}' \phi(x) \partial_{x'} \Delta_H(x-x') \partial_{x'} \phi(x') \bigg|_{t=t'}. \]

The probability density \( J_0^P(x) \) is not Lorentz invariant, which is especially clear from the position space expression in equation \cite{80}. The probability density current \( J^P_{\mu}(x) \) is, however, Lorentz covariant. Also, the normalization of our probability to one, where \( J^P_{\mu}(x) \) is integrated over its entire domain, is Lorentz invariant. The reason is that the inner product integral contains a Lorentz covariant vector valued volume element, which contracts with the current to give a Lorentz invariant result.
The probability current \( J^\mu_P(x) \) in equation (78) merits a final remark. For real fields, we have that \( \phi_-(x) = \phi^*_+(x) \). Clearly, the probability current is in that case equal to the ordinary Klein Gordon current, given by:

\[
N^KG_\mu(x) = \phi^*_+(x)i\overset{\leftarrow}{\partial}_\mu\phi_+(x),
\]

where the negative frequency contributions in (78) are mapped to the positive frequency Hilbert space. Therefore, equation (87) is a probability density too. Such an interpretation can for example be found in [17, 18, 34]. Although \( J^\mu_P(x) \) and \( N^KG_\mu(x) \) are equal, there are profound differences between the dynamics of the wave function \( \phi(x) \), which is causal, and of \( \phi_+(x) \), which is not causal. Therefore, the positive frequency contribution to the real field on its own cannot be a relativistic wave function.

\[\text{B. Particle Interpretation}\]

In non-relativistic quantum mechanics, a wave function describes the probability density of a single particle. Motivated by the discussion above, it is natural to interpret the probability density in equation (80) as the number density for a single particle too:

\[
N = \frac{1}{2}\langle\phi|\phi\rangle = \frac{1}{2}\int d^3\vec{x}\phi^*_+(x)i\overset{\leftarrow}{\partial}_0\phi_+(x) - \phi^*_+(x)i\overset{\leftarrow}{\partial}_0\phi_-(x) = 1.
\]

In other words, it is the superposition of positive and negative frequency wave packets, normalized to unity, that defines one particle. Hence, our particle interpretation is in agreement with the particle interpretation as advocated in non-relativistic quantum mechanics. Take for example the Gaussian ground state of a simple harmonic oscillator. Clearly, it consists of the superposition of many wave modes but is nevertheless generally regarded as a single particle quantum mechanical wave function. This differs from the particle interpretation that is usually adhered to in quantum field theory, where one mode \( |k\rangle = \hat{a}_k^\dagger|0\rangle \) is interpreted as one particle, see e.g. [49]. It also differs from various claims made in the literature that the wave function for a single relativistic particle does not exist in quantum field theory\[11\] [15, 20, 44, 46].

The particle number in the sense defined above in equation (88) is only conserved in free theories. As for the electric charge density, and for the probability density, we can define a Lorentz covariant

\[\text{\text{\textsuperscript{11}We are able to adhere to a single particle wave function interpretation since in our framework wave functions propagate causally. As mentioned before however, there are still problems related to non-locality in the standard treatments of position operators. This issue will be resolved in [21].}}\]
particle density current:

\[ N_\mu = \frac{1}{2} \phi^+_\mu(x) i \gamma_\mu \phi_+(x) - \frac{1}{2} \phi^-_\mu(x) i \gamma_\mu \phi_-(x). \]  
(89)

For complex fields for instance the charge current and the energy momentum current are conserved because the Lagrangian following from (5) is invariant under \( U(1) \) and it is translationary invariant. The particle number density current defined in equation (89) is not protected by such a symmetry in interacting theories.

**IV. CAUSAL PROPAGATION OF QUANTUM FIELDS**

**A. The Hadamard Composition Law and the Wheeler Propagator**

In the previous sections, we have developed a first quantized picture for free scalar quantum field theories. In this final section, we rigorously show that probabilities, defined in e.g. equation (86) where we made use of the Hadamard propagator, propagate causally.

Let us firstly remind the reader again that the Feynman propagator is not a causal propagator. Suppose that, at some initial time \( t' \), one specifies a certain state \( |\phi\rangle \), defined in equation (22a).

Let us now recall equation (48a):

\[ \theta(t - t') \phi_+(x) = \int d^3 \vec{x}' \Delta_F(x - x') \gamma^\nu \phi_+(x'). \]

The Feynman propagator has a non-vanishing support outside the past and future light cone of \( x' \) and hence we see that it propagates the positive frequency contribution to our real field \( \phi \) instantaneously outside the future light cone of its region of non-zero support. The Wheeler propagator stems from the commutator, and thus only has non-vanishing support inside the past and future light cone of \( x' \). If we recall equation (68):

\[ \epsilon(t - t') \phi(x) = \int d^3 \vec{x}' \Delta_W(x - x') \gamma^\nu \phi(x'), \]

we conclude that \( \phi(x) \) will only be non-zero if \( x \) is the past or future light cone of the region of non-zero support of \( \phi(x') \). Qualitatively, this is depicted in figure I.

The probability for some observer for finding a particle in some spacelike region \( A \), can be calculated by making use of the Hadamard propagator, as we recall from equation (86):

\[ P = \frac{1}{2} \left| \int_A d^3 \vec{x} d^3 \vec{x}' \phi(x) \gamma^\nu \Delta_H(x - x') \gamma^\nu \phi(x') \bigg|_{t=t'} \right|. \]
Figure 1: Qualitative picture of the causal propagation of a quantum field mediated by the Wheeler propagator. Note that the evolution ensures that no contributions propagate beyond the causal region of the initial state. In other words, outside the causal future of the wave packet there is perfect destructive interference between the positive and negative frequency modes.

We can derive the following composition law for the Hadamard propagator:

$$-\frac{1}{4} \phi(t - t_y) \phi(t' - t_{y'}) \Delta_H(x - x') = \int d^3 \vec{y} d^3 \vec{y}'' \Delta_W(x - \vec{y}) \partial_{t_y} \Delta_H(y - y') \partial_{t_{y'}} \Delta_W(y' - x').$$  \hspace{1cm} (90)

Here, we made use of equations (56) and (70). We have thus expressed the Hadamard composition law in terms of the Wheeler propagator rather than the commutator propagator as in equation (84). Also, we defined $y = (y_t, \vec{y})$. Alternatively, we can absorb the minus sign in front of equation (90) in the composition law as follows:

$$\frac{1}{4} \phi(t - t_y) \phi(t' - t_{y'}) \Delta_H(x - x') = \int d^3 \vec{y} d^3 \vec{y}'' \Delta_W(x - \vec{y}) \partial_{t_y} \Delta_H(y - y') \partial_{t_{y'}} \Delta_{AW}(y' - x'),$$ \hspace{1cm} (91)

where the anti-Wheeler propagator is defined as the anti-time ordered commutator propagator:

$$\Delta_{AW}(x - x') = \frac{1}{2} T \Delta_C(x - x') = -\Delta_W(x - x').$$ \hspace{1cm} (92)
If both $t$ and $t'$ are later than $t_y$ and $t_{y'}$, the composition law takes a rather neat form:

$$\Delta H(x - x') = 4 \int d^3y' d^3y'' \Delta_W(x - y) \hat{\partial}_{t_y} \Delta_H(y - y') \hat{\partial}_{t_{y'}} \Delta_{AW}(y' - x') \{ (t', t') > t_y \} \{ (t', t') > t_{y'} \}.$$

We already showed before that the Wheeler propagator governs the causal dynamics of the entire wave function $\phi(x)$. Now, together with equation (93) shows explicitly that probabilities propagate causally too as the time evolution of the Hadamard propagator can be expressed solely in terms of the causal Wheeler propagator. A final technical remark is in order. The factor of 4 that appears on the right hand side in equation (93) arises from our definition of the Wheeler propagator as a factor of half times the time ordered commutator, such that the Wheeler propagator is a Green’s function. If we would not have inserted the factor of $1/2$ in our definition, the Hadamard propagator would satisfy a neater looking composition law.

### B. Example I: a Localized Wave Function

In order to illustrate the discussion above, let us study the propagation of two wave packets: a specific $\phi_+(x)$ and $\phi(x)$. We consider the following wave function $\phi$:

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2} \left[ e^{ik_+ (x - x')} + e^{ik_- (x - x')} \right].$$

We have thus chosen the following wave packet:

$$\phi(k_\pm) = \omega_k e^{-ik_{\pm} x'},$$

The second wave packet we wish to consider is $\phi_+(x)$ which can be read off from equation (94):

$$\phi_+(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2} e^{ik_+ (x - x')}.$$

These wave packets do not give rise to a probability density that can be normalized according to equation (94). The reason for introducing these wave packets nevertheless is that they are perfectly localized initially:

$$\phi(x)|_{t=t'} = \delta^3(\vec{x} - \vec{x}')$$

$$\phi_+(x)|_{t=t'} = \frac{1}{2} \delta^3(\vec{x} - \vec{x}').$$

These (extremely well) localized wave packets allow for a clean comparison between the form of the wave packets for $t > t'$. The conventional Newton-Wigner wave packet [47] is not given by equation (95) but rather by:

$$\phi_{NW}^+(k) = \omega_k^2 e^{-ik_{+} x'},$$
and, consequently, gives rise to a wave function that is not perfectly localized initially. In fact, the position space expression for the Newton-Wigner wave packet yields at $t = t'$:

$$
\phi_{NW}^{\ast}(x) = \frac{1}{2\pi^3 \Gamma \left( \frac{3}{4} \right)} \left( \frac{m}{\| \vec{x} - \vec{x}' \|} \right)^{\frac{3}{4}} K_{\frac{3}{4}} \left( m \| \vec{x} - \vec{x}' \| \right),
$$

where $K_{\nu}(x)$ is a modified Bessel function of order $\nu$. This expression reveals that the Newton-Wigner wave packet is not perfectly localized initially.

All we need to do next, is perform the Fourier integrals in (94) and (96). We make use of the form of the two Wightman propagators (35) and introduce two $\epsilon$ pole prescriptions to regulate the integral. Let us for simplicity consider a massless field such that $\omega_k = \| \vec{k} \|$. Our wave function is given by:

$$
\phi(x) = \zeta^\mu \partial_{\mu} \left[ \Delta^+(x - x') + \Delta^-(x - x') \right] = \partial_t \left[ \Delta^+(x - x') + \Delta^-(x - x') \right]
$$

(100)

In the first equality we have chosen our state such that $\zeta^\mu$ is normal to the spatial hypersurface. Moreover, the equations on the second and third line are to be interpreted in the distributional sense where $\epsilon \to 0$. Most importantly, our wave packet spreads in time and gives a non-vanishing contribution only on the light cone. This is to be contrasted with the result for $\phi_+^\ast(x)$ which results from propagation forward in time with the Feynman propagator:

$$
\phi_+(x) = \partial_t \Delta^+(x - x') = \frac{i(t - t')}{2\pi^2 \left[ -(t - t' - i\epsilon)^2 + \| \vec{x} - \vec{x}' \|^2 \right]}.
$$

(101)

This wave packet has non-vanishing contributions outside the light cone too. We conclude that although initially both wave packets are extremely well localized as delta functions, at later times spreading of the wave packets has occurred such that our wave function $\phi(x)$ has a non-vanishing contribution only on the light cone whereas $\phi_+(x)$ has not propagated in such a causal manner and has a non-vanishing contribution outside the light cone too. This example thus shows that only $\phi(x)$ can be a wave function consistent with the relativistic principle of causality.

### C. Example II: a Localized Probability Density

We can also consider relativistic wave packets that can be properly normalized according to equation (76). Let us now consider another wave function $\phi(x)$ which is given by:

$$
\phi(x) = \frac{1}{\sqrt{N}} \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[ e^{ik_+(x-x'-i\xi)} + e^{ik_-(x-x'+i\xi)} \right].
$$

(102)
Note that with this normalization \( \phi(x) \) and \( \mathcal{N} \) are Lorentz scalars. This time, we have thus chosen the following wave packet [48]:

\[
\phi(k_{\pm}) = \frac{1}{\sqrt{\mathcal{N}}} e^{-i k_{\pm} (x' \pm i \xi)}, \tag{103}
\]

where \( \xi \) is a timelike vector with \( \xi^0 > \|\xi\| \) such that the momentum space integral converges and where \( \mathcal{N} \) is a normalization constant. For simplicity we will consider \( \xi^\mu = (\epsilon, 0, 0, 0) \) only. In particular, we will be interested in the limit where \( \epsilon \) is small. In principle, however, we can generalize this analysis to more general states where \( \xi^0 \) is arbitrarily large and where \( \|\xi\| \neq 0 \) as long as the convergence condition \( \xi^0 > \|\xi\| \) is satisfied. Physically, states with \( \|\xi\| \neq 0 \) have a non-zero initial velocity of the wave packet. Also, \( \xi_0 \) determines the width of the wave packet. It is interesting to note that for \( m \neq 0 \), \( x' = 0 \) and for small \( \|k\| \) the wave packet in equation (103) is a Gaussian. For a more general discussion of the dynamics of wave packets, see [21]. Let us again specialize to massless scalar fields for which \( \omega_k = \|k\| \). We can normalize our state by making use of equation (76):

\[
\mathcal{N} = \frac{1}{(4\pi \epsilon)^2}. \tag{104}
\]

We can evaluate the Fourier integrals that appear in equation (102) to find our wave function in position space:

\[
\phi(x) = \frac{\epsilon}{\pi \left[-(t - t' - i\epsilon)^2 + \|\vec{x} - \vec{x}'\|^2\right]} + \frac{\epsilon}{\pi \left[-(t - t' + i\epsilon)^2 + \|\vec{x} - \vec{x}'\|^2\right]}. \tag{105}
\]

We are interested in the probability density which we defined earlier in equation (80):

\[
\rho_P(x) = \frac{4\epsilon^3 \left[(t - t')^2 + \|\vec{x} - \vec{x}'\|^2 + \epsilon^2\right]}{\pi^2 \left[-(t - t' - i\epsilon)^2 + \|\vec{x} - \vec{x}'\|^2\right]^2 \left[-(t - t' + i\epsilon)^2 + \|\vec{x} - \vec{x}'\|^2\right]^2}. \tag{106}
\]

As a simple computational check of the normalization of our probability density, one can easily verify that:

\[
\int d^3\vec{x} \rho_P(x) = 1, \tag{107}
\]

for arbitrary times as it should. In figure [2] we show the real wave function in equation (105) at two different times. In ordinary quantum mechanics, one cannot so easily visualize the wave function as it is complex valued. In figure [3] we show the resulting probability density in equation (106). Note that it is a spherical wave travelling at the speed of light. The reason for considering a wave function of the form (102) is that initially its corresponding probability distribution is extremely well localized:

\[
\rho_P(x)|_{t=t'} = \frac{4\epsilon^3}{\pi^2 \left[\epsilon^2 + \|\vec{x} - \vec{x}'\|^2\right]^3}. \tag{108}
\]
Sending $\epsilon$ to zero yields:

$$\lim_{\epsilon \to 0} \rho_P(x)|_{t'=t} = \frac{1}{2\pi \| \vec{x} - \vec{x}' \|^2} \delta(||\vec{x} - \vec{x}'||) = \delta^{(3)}(\vec{x} - \vec{x}') .$$

(109)

Interestingly, the probability density for $t - t' > 0$ is given by:

$$\lim_{\epsilon \to 0} \rho_P(x) = \frac{1}{4\pi \| \vec{x} - \vec{x}' \|^2} \left[ \delta \left( \| \vec{x} - \vec{x}' \| - (t - t') \right) + \delta \left( \| \vec{x} - \vec{x}' \| + (t - t') \right) \right] .$$

(110)

For massless scalar fields, we thus observe that the probability density propagates exactly on the light cone. Furthermore, it is important to realize that although $\phi_+(x)$ evolves with the Feynman propagator and consequently spreads outside the light cone of its initial region of non-zero support, the probability density at late times behaves perfectly causal. The reason is that our probability density given in equation (80) and the Klein Gordon current in equation (87) are equal. This is of course not surprising. The reason for introducing the Wheeler propagator and real valued relativistic wave functions has not been to prove causality at the level of probabilities as expectation values in quantum field theory are already perfectly causal. The main point of our formalism, however, is that in-out amplitudes themselves can be treated causally too. Finally, we would like to stress that our single particle real valued relativistic wave function in equation (102) is localized and can be properly normalized. This is to be contrasted with the states constructed by Newton and Wigner [47] as the eigenstates of the Newton-Wigner position operator.
V. CONCLUSION

We have carefully developed a first quantized interpretation for real scalar fields in non-interacting scalar field theory:

- The wave function of quantum field theory is the entire real field \( \phi(x) \), which generalizes the wave function of non-relativistic quantum mechanics;

- The dynamics of the wave function is governed by the Klein Gordon equation, which generalizes the Schrödinger equation in quantum mechanics;

- The probability density follows from the innerproduct on the Hilbert space of positive and negative frequency contributions to \( \phi(x) \). The probability density is of course normalized to unity when integrated over its domain of non-zero support.

By making use of the stress-energy tensor for a real field we also showed that the negative frequency solutions have positive energy. The particle interpretation made in a first quantized picture of quantum field theory differs from the particle interpretation that is usually advocated in quantum field theory. We interpret a wave function normalized to unity as the quantum mechanical wave function of a single particle. Due to the superposition principle, this wave packet thus contains many wave modes. In conventional quantum field theory, one wave mode is usually interpreted as one particle, see for instance [49]. The dynamics of the single particle wave function \( \phi(x) \) is governed by the Wheeler propagator, which is the time ordered commutator propagator. The Wheeler propagator has several advantages when compared to the Feynman propagator:

- Unlike the Feynman propagator, the Wheeler propagator is causal. It does not have any contributions outside of the past and future light cones of its arguments \( x \) and \( x' \);

- The Wheeler propagator is real and propagates the entire real field \( \phi(x) \), while the Feynman propagator is complex valued and only propagates the positive frequency contribution \( \phi_+(x) \);

- Both the Wheeler and the Feynman propagator are Green’s functions, which makes them particularly convenient to develop perturbation theory. However, only the Wheeler propagator is the Green’s function of the entire real field \( \phi \).

Precisely because the Wheeler propagator or the commutator propagator governs the causal propagation of the real field \( \phi(x) \), we can interpret the field itself as the wave function in relativistic...
quantum mechanics. This is to be contrasted with the function $\phi_+(x)$ that is virtually instantaneously propagated outside the past or future light cone of its region of non-zero support by the Feynman propagator.

In our approach the probabilities are calculated using the Hadamard propagator. We only need the equal time Hadamard propagator, so it plays no role in the dynamics of our scalar field. The Hadamard propagator satisfies a composition law that can be expressed solely in terms of the Wheeler propagator. We have thus shown that probabilities in our form of the in-out formalism propagate causally. In other words: causality is restored in the in-out formalism of quantum field theory by properly including the negative frequency solutions to the Klein Gordon equation.

We would also like to mention again that expectation values of observables in the first quantized picture of quantum field theory will not be affected by whether one makes use of the Feynman propagator or of the Wheeler propagator to calculate them. So, standard quantum field theory in the in-out formalism is causal when expectation values of observables are considered, but not when amplitudes are calculated. However, by making use of the Wheeler propagator, we have been able to implement causality explicitly at the level of the dynamics of the fields, unlike in the conventional picture of first quantized quantum field theory.

The first quantized picture of quantum field theory we discussed here is only complete if we can derive a local position operator. This issue will be addressed in a separate publication [21]. As said at various places throughout the paper, we have only considered free real scalar fields. Of course, we are in the process of generalizing our setup to interacting scalar fields and set up a perturbative expansion using the Wheeler propagator to calculate expectation values. Also, it would be very interesting to generalize our setup to e.g. de Sitter spacetime.

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