The scalar field kernel in cosmological spaces

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Received 24 January 2008, in final form 15 April 2008
Published 2 June 2008
Online at stacks.iop.org/CQG/25/125009

Abstract
We construct the quantum-mechanical evolution operator in the functional Schrödinger picture—the kernel—for a scalar field in spatially homogeneous FLRW spacetimes when the field is (a) free and (b) coupled to a spacetime-dependent source term. The essential element in the construction is the causal propagator, linked to the commutator of two Heisenberg picture scalar fields. We show that the kernels can be expressed solely in terms of the causal propagator and derivatives of the causal propagator. Furthermore, we show that our kernel reveals the standard light cone structure in FLRW spacetimes. We finally apply the result to Minkowski spacetime, to de Sitter spacetime and calculate the forward time evolution of the vacuum in a general FLRW spacetime.

PACS numbers: 98.80.−k, 98.80.Jk, 04.62.+v, 03.65.Db

1. Introduction

The functional Schrödinger picture is based on the projection of quantum states and operators on the field amplitude basis. Guth and Pi [1] have already used it in the study of inflationary perturbations and related the width of the Gaussian vacuum wavefunctional in de Sitter spacetime to Heisenberg picture scalar fields, thus casting quantum field theory in terms familiar from non-relativistic quantum mechanics.

A kernel is a quantum-mechanical evolution operator in the functional Schrödinger picture and is the fundamental object of any quantum-mechanical theory. It represents a transition amplitude from an arbitrary initial state at time \( t' \) to an arbitrary final state at time \( t \). Moreover, it allows us to calculate the forward time evolution of any given initial field configuration. In this paper, we demonstrate that the kernel can be expressed solely in terms of the causal propagator and derivatives of the causal propagator thus elaborating further on the connection

\[ \text{Note that in some of the literature this object is referred to as the quantum-mechanical propagator.} \]
with the Heisenberg (operator) picture for quantum field theories. Furthermore, the appearance of the causal propagator makes the causality structure of the theory evident.

The kernel allows for many physical applications in quantum field theory. For example, if interactions between various scalar fields or fermionic fields are linear in (one of the) matter fields, the formalism developed here can straightforwardly be applied. Furthermore, another natural application of the kernel can be found in the study of decoherence [2, 3] accounting for the quantum-to-classical transition in the early universe.

After having reviewed some basic quantum mechanics in the current section, we will calculate the kernel for a free scalar field in section 2, and a scalar field coupled to a source term in section 3 in cosmological spacetimes (spatially homogeneous backgrounds). In section 4 we elaborate on causality in quantum field theory expressed in the functional Schrödinger picture and end in section 5 with some examples, to wit, the simple harmonic oscillator, the kernel in de Sitter spacetime and the time evolution of the vacuum state in Friedmann–Lemaître–Robertson–Walker or FLRW spacetimes.

1.1. Essentials from quantum mechanics

Let us begin by recalling some basic identities from quantum mechanics. A quantum state |Ψ(t)⟩ at time t can in general be expressed in terms of the evolution operator ˆU(t, t′) and the quantum state |Ψ(t′)⟩ at initial time t′ as follows:

|Ψ(t)⟩ = ˆU(t, t′)|Ψ(t′)⟩.  \(\text{(1)}\)

Just as the state |Ψ(t)⟩, the evolution operator ˆU(t, t′) obeys the Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} \hat{U}(t, t') = \hat{H} \hat{U}(t, t'), \]

where ˆH is the Hamiltonian operator of the system under consideration. The formal solution is a time-ordered (T) exponential,

\[ \hat{U}(t, t') = T \exp \left( -\frac{i}{\hbar} \int_{t'}^{t} dt'' \hat{H}(t'') \right). \]

(3)

Note that t > t′ is implied and when t < t′ time ordering should be replaced with anti-time ordering (T). From this equation, we can easily infer some important properties which the evolution operator satisfies

\[ \hat{U}^\dagger(t, t') = \hat{U}(t', t) \] \(\text{(4a)}\)

\[ \hat{U}(t', t') = 1 \] \(\text{(4b)}\)

\[ \hat{U}(t, t'') \hat{U}(t'', t') = \hat{U}(t, t') \] \(\text{(4c)}\)

1.2. Expectation values and commutators

Let us now state a relation between quantum-mechanical expectation values and commutators (see, for example, [4]) which will play an important role in the interpretation of the kernel.

We consider the expectation value of some general operator ˆQ in the Schrödinger picture

\[ \langle \hat{Q}(t) \rangle = \langle \Psi(t)|\hat{Q}|\Psi(t)\rangle. \]

(5)

Now, by using (3) for the evolution operator,

\[ \langle \hat{Q}(t) \rangle = \langle \Psi(t')| \left\{ T \exp \left( -\frac{i}{\hbar} \int_{t'}^{t} dt'' \hat{H}(t'') \right) \right\} \hat{Q} \left\{ T \exp \left( \frac{i}{\hbar} \int_{t}^{t'} dt'' \hat{H}(t'') \right) \right\} |\Psi(t')\rangle. \]

(6)
one can prove by induction that at each order in \( \hat{H} \) one has
\[
\langle \hat{Q}(t) \rangle = \sum_{n=0}^{\infty} \left( \frac{i}{\hbar} \right)^n \int_{t}^{t'} dt_n \int_{t'}^{t_{n-1}} dt_{n-1} \cdots \int_{t_n}^{t_{n-1}} dt_2 \int_{t_2}^{t_1} dt_1 \langle \Psi(\hat{t}_1) | [\hat{H}(\hat{t}_1), [\hat{H}(\hat{t}_2), \cdots [\hat{H}(\hat{t}_n), \hat{Q}] \cdots ] | \Psi(\hat{t}_1) \rangle.
\] (7)

We can conclude that expectation values, naturally defined in terms of evolution operators as in (6), can in a fully equivalent manner be calculated from the expectation value of nested commutators, as in (7). Information about observables is hence equally well stored in a series of commutators as in evolution operators.

In quantum-mechanics causality corresponds to the statement that all commutators of observables, including non-commuting observables, vanish outside past and future light cones. Alternatively, measurements performed at points in spacetime with a spacelike separation can be carried out simultaneously. This equivalence relation already suggests that quantum mechanics is a causal theory in full generality since, up to higher order irreducible \( n \)-point functions, expectation values can be expressed in terms of the commutator, a manifestly causal quantity. These are vital observations, and we will return to them shortly.

1.3. The causal propagator

Given some quantum field operator \( \hat{\phi}(x) \) in the Heisenberg picture one can construct various vacuum expectation values by means of the Schwinger–Keldysh formalism (see, e.g., [5]). We will be interested in a particular linear combination of the two Wightman functions (\( G_{++} \) and \( G_{--} \)) to construct what we will henceforth refer to as the causal propagator
\[
G_c(x, x') = G_{--}(x, x') - G_{+-}(x, x') = \langle \Omega | [\hat{\phi}(x), \hat{\phi}(x')] | \Omega \rangle = \langle \Omega | \hat{\phi}(x)\hat{\phi}(x') - \hat{\phi}(x')\hat{\phi}(x) | \Omega \rangle.
\] (8)

In particular, if we assume a spatially homogeneous background and a quadratic Hamiltonian, expanding in terms of creation and annihilation operators
\[
\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3} \hat{a}_k \phi_k(t) e^{ik \cdot x} + \hat{a}_k^\dagger \phi_k^*(t) e^{-ik \cdot x},
\] (9)
yields
\[
G_c(x, x') = \hbar \int \frac{d^3k}{(2\pi)^3} G_c(k, t, t') e^{ik \cdot (x-x')},
\] (10)
where
\[
G_c(k, t, t') = \phi_k(t)\phi_k^*(t') - \phi_k^*(t)\phi_k(t').
\] (11)

Here, the \( \hbar \) originates from imposing the standard commutation relations between creation and annihilation operators. Furthermore, note the field modes are homogeneous, i.e., \( \phi_k(t) \) depends on \( k = ||k|| \).

This propagator is causal in the quantum-mechanical sense because it originates from the commutator [6], unlike for example the Feynman or (anti-)time ordered propagators.

1.4. The functional Schrödinger picture

In the functional Schrödinger picture [1, 7–9] a quantum-mechanical state \( |\Psi(t)\rangle \) is realized by a wavefunctional \( \Psi(\phi, t) \) which is a functional of the \( c \)-number functions \( \phi = \{\phi(x), \forall x \in \mathbb{R}^3\} \) defined by the projection on the field amplitude basis \( \Psi(\phi, t) = \langle \phi | \Psi(t) \rangle \), where
The action of a quantum field operator $\hat{\phi}(x)$ and its associated canonical momentum $\hat{\pi}(x)$ are given by

$$\langle \phi | \hat{\phi}(x) | \Psi(t) \rangle = \phi(x) \Psi(\phi, t)$$

(12)

$$\langle \phi | \hat{\pi}(x) | \Psi(t) \rangle = \frac{\hbar}{i} \frac{\delta}{\delta \phi(x)} \Psi(\phi, t).$$

(13)

2. The kernel for the free scalar field

Let us now examine the quantum-mechanical evolution operator (3) in the functional Schrödinger picture

$$K(\phi, t; \phi', t') \equiv \langle \phi | \hat{U}(t, t') | \phi' \rangle = \int D\phi'' K(\phi, t; \phi'', t'') K(\phi'', t''; \phi', t'),$$

(14)

where $K$ is the so-called kernel, a transition amplitude from some initial state $\phi'$ at $t'$ to the state $\phi$ at $t$. The kernel can be expressed in terms of a path integral of the action where we integrate over all intermediate field configurations.

It is interesting to note that from properties (4) we deduce the following symmetry requirements for $K$:

$$K^*(\phi, t; \phi', t') = K(\phi', t'; \phi, t)$$

(15a)

$$K(\phi, t; \phi', t) = \delta(\phi - \phi')$$

(15b)

$$K(\phi, t; \phi', t') = \int D\phi'' K(\phi, t; \phi'', t') K(\phi'', t''; \phi', t'),$$

(15c)

where the functional delta function has to be understood as $\delta(\phi - \phi') = \prod_x \delta(\phi(x) - \phi'(x))$.

The action for a real scalar field $\phi(x)$ for a finite time interval ranging between $t'$ and $t$ generally valid for real quantum fields in curved spacetimes is given by

$$S[\phi] = \int d^4x \sqrt{-g} \left( -\frac{1}{2} \partial_\mu \phi(x) \partial^\mu \phi(x) g^{\alpha\beta} - \frac{1}{2} (m^2 + \xi R) \phi^2(x) \right),$$

(16)

where $R$ denotes the Ricci curvature scalar and $g = \det[g_{\mu\nu}]$. Let us specialize to FLRW spacetimes in which the metric is given by $g_{\mu\nu} = \text{diag}(-1, a^2(t), a^2(t), a^2(t))$ where $a(t)$ is the scale factor of the universe. Classically, this action leads to the standard equation of motion

$$\Box \phi_{cl}(x) - (m^2 + \xi R) \phi_{cl}(x) = 0,$$

(17)

where $\Box = (-g)^{-1/2} \partial_\mu (-g)^{1/2} g^{\mu\nu} \partial_\nu$ is the scalar d’Alembertian. We write

$$\phi(x) = \phi_{cl}(x) + \delta\phi(x),$$

(18)

and insert this into equation (16). The boundary conditions on $\phi(x)$ are carried by the classical field only, i.e., $\phi_{cl}(x, t') = \phi'(x)$ and $\phi_{cl}(x, t) = \phi(x)$, and straightforwardly result into the requirement that $\delta\phi(x, t') = 0 = \delta\phi(x, t)$. Assuming that the classical field (17) vanishes at spatial infinity, two straightforward partial integrations yield

$$S[\phi_{cl} + \delta\phi] = S[\delta\phi] + S[\phi_{cl}] = S[\delta\phi] + \frac{1}{2} \int d^3x \phi_{cl}(x) \pi_{cl}(x),$$

(19)
where we have recognized the canonical momentum associated with $\phi(x)$ given by $\pi_{\phi}(x) = a(t) \phi(x)$. Equation (14) boils down to the following result:

$$K(\phi, t; \phi', t') = \exp\left[\frac{i}{\hbar} \int d^3 x \phi(x) \pi_{\phi}(x) \right]_{\phi(t)}^{\phi(t') = 0} \delta \phi \exp\left[\frac{i}{\hbar} S[\phi] \right].$$

(20)

Note that the remaining path integral represents the transition amplitude between zero field states and is thus independent of the original boundary conditions on the field $\phi(x)$. Hence we can absorb this factor into the overall normalization of the kernel

$$K(\phi, t; \phi', t') = \mathcal{M}(t, t') \exp\left[\frac{i}{\hbar} \int d^3 x \phi(x) \pi_{\phi}(x) \right]_{\phi(t)}^{\phi(t') = 0} \delta \phi \exp\left[\frac{i}{\hbar} S[\phi] \right].$$

(21)

Next, we Fourier expand the classical field

$$\phi(x) = \int \frac{d^3 k}{(2\pi)^3} \phi(k) e^{ikx},$$

which is well defined because we consider a spatially flat FLRW background. Note the property $\phi^*_{\phi}(t) = \phi_{-k}^*(t)$ and the omission of the subscript ‘cl’ of the field modes for future convenience. We must keep in mind, though, that also the field modes are classical in the sense that they obey the Fourier transform of equation of motion (17),

$$\left(\frac{\partial^2}{\partial t^2} + 3H \frac{\partial}{\partial t} + \frac{k^2}{a^2(t)} + m^2 + \xi R \right) \phi_k(t) = 0,$$

(23)

where $H(t) = \dot{a}(t)/a(t)$ is the Hubble parameter. We thus have

$$S[\phi_{cl}] = \frac{1}{4} \int \frac{d^3 k}{(2\pi)^3} |a^3(t) \partial_t |\phi_k(t)|^2| \right|_{\text{full}}.$$

(24)

Note that running time $\bar{t}$ is defined on the interval $t' \leq \bar{t} \leq t$. Let us denote the two fundamental solutions of (23) by $\chi_k(\bar{t})$ and $\chi_k^*(\bar{t})$. In general, $\phi(\bar{t})$ is a linear superposition of the two fundamental solutions, i.e., $\phi_{\bar{t}}(\bar{t}) = \alpha_k \chi_k(\bar{t}) + \beta_k \chi_k^*(\bar{t})$. We are now in the position to impose the boundary conditions at initial and final times and solve for $\alpha_k$ and $\beta_k$. We thus find

$$\phi_{\bar{t}}(\bar{t}) = \phi_k G_{k}(\bar{t}, t') + \phi_k^* G_{k}^*(\bar{t}, t'),$$

(25)

where $G_k(t, t')$ is related to the causal propagator (11) as follows:

$$G_k(t, t') = \phi_k(t) \phi_k^*(t') - \phi_k^*(t) \phi_k(t') = G_k(k, t, t') \text{sgn}(\mathbf{k} \cdot \mathbf{n}),$$

(26)

where $\mathbf{n}$ is a unit vector in k-space normal to an arbitrary plane through the origin. The sign-function is introduced in order to preserve the odd symmetry under $\mathbf{k} \rightarrow -\mathbf{k}$. One can thus express the solution to differential equation (23) in terms of its boundary conditions and causal propagators exclusively. We believe that this is also true for general spacetimes and fields of nonzero spin [10].

Note that the Wronskian yields

$$W[\phi_k(t), \phi_k^*(t)] = \phi_k(t) \phi_k^*(t) - \phi_k^*(t) \phi_k(t) = (|\alpha_k|^2 - |\beta_k|^2) W[\chi_k(t), \chi_k^*(t)],$$

(27)

where

$$|\alpha_k|^2 - |\beta_k|^2 = \frac{1}{G_k(t, t')} (\phi_k \phi_k^* - \phi_k^* \phi_k).$$

(28)

Generally, this equation does not equal unity, a requirement usually imposed for a consistent canonical quantization in the Heisenberg picture, because the boundaries are arbitrary. Indeed, this is an important difference between the Schrödinger and Heisenberg pictures.
Next, we substitute (25) into our modified action, equation (24). The finite volume (in position space) result for the kernel in Fourier space reads

\[ K(\phi, t; \phi', t') = \prod_k M_k \exp \left[ -\frac{i}{V} \left( B(k, t, t')\phi_k\phi_k^* + C(k, t, t')\phi_k^*\phi' + \frac{1}{2} D(k, t, t') (\phi_k\phi_k^* + \phi_k^*\phi'_k) \right) \right], \]  

(29)

where \( M_k \) is a normalization constant and where

\[ B(k, t, t') = -\frac{ia^3(t)}{2\hbar} \frac{\partial}{\partial k} G_k(t, t') \]  

(30a)

\[ C(k, t, t') = \frac{ia^3(t')}{2\hbar} \frac{\partial}{\partial k} G_k(t, t') \]  

(30b)

\[ D(k, t, t') = -\frac{i}{2\hbar G_k(t, t')} \left\{ a^3(t)W[\chi_k(t), \chi_k^*(t)] + a^3(t')W[\chi_k(t'), \chi_k^*(t')] \right\}. \]  

(30c)

Note that \( B(k, t, t') = B(k, t, t') \) due to the homogeneity of space. The volume factor appearing in (29) is due to the identification \( \int \frac{dk}{(2\pi)^3} = \frac{1}{V} \sum_k \) valid in the infinite volume limit, which we use throughout this paper. In FLRW spacetimes, the Wronskian equals

\[ W[\chi_k(t), \chi_k^*(t)] = \frac{i}{a^3(t)} \text{sgn}(k \cdot \mathbf{n}). \]  

(31)

Note again the appearance of the sign-function.

Finally, the appropriate normalization constant can be determined upon inserting the kernel (29)–(30) into the functional Schrödinger equation

\[ \left( i\hbar \partial_t - \int d^3x \frac{-\hbar^2}{2a^3(t)} \frac{\delta^2}{\delta \phi^*(x)} + \frac{a(t)}{2} \left( \nabla \phi(x) \right)^2 + \frac{a^3(t)}{2}(m^2 + \xi R)\phi^2(x) \right) K(\phi, t; \phi', t') = 0. \]  

(32)

We consider the following general form for the kernel (29) in position space:

\[ K(\phi, t; \phi', t') = M(t, t') \exp \left[ -\int d^3y d^3z [\phi(y)\phi(z)B(y, z) + \phi'(z)\phi'(z)C(y, z) + \phi(y)\phi'(z)D(y, z)] \right], \]  

(33)

where we define for example \( B(y, t; z, t') \equiv B(y, z) \) for brevity and where

\[ B(y, z) = \int \frac{d^3k}{(2\pi)^3} B(k, t, t') e^{ik \cdot (y-z)}, \]  

(34)

and similarly for \( C(y, z) \) and \( D(y, z) \). Using (30), we can easily check that the Fourier transform of (33) satisfies the functional Schrödinger equation at each (nonzero) order in the fields \( \phi \) and \( \phi' \). At zeroth order, the functional Schrödinger equation reads

\[ i\hbar \frac{\partial}{\partial t} \log M(t, t') - \frac{\hbar^2}{a^3(t)} \int d^3x B(x, x) = 0. \]  

(35)

After switching to Fourier space, we write \( M(t, t') = \prod_k M_k(t, t') \). Next, it is a non-trivial step to exploit the functional Schrödinger equation at order \( \phi\phi' \) in order to explicitly preserve the invariance under \( k \rightarrow -k \). This yields

\[ i\hbar \frac{\partial}{\partial t} \log M_k(t, t') = -\frac{i\hbar}{2} \frac{\partial}{\partial t} \log D(k, t, t') = 0. \]  

(36)
We can solve this differential equation straightforwardly,

\[ \mathcal{M}_k(t, t') = \mathcal{M}_{0,k} \sqrt{D(k, t, t')}, \]

where the time-independent constant \( \mathcal{M}_{0,k} \) has to be fixed by condition (15b), or, alternatively by requiring \( \int D\phi K(\phi, t; \phi', t) = 1 \). The result is \( \mathcal{M}_{0,k} = 1/\sqrt{-2\pi V} \). Hence, the normalization constant is given by

\[ \mathcal{M}_k(t, t') = \sqrt{-D(k, t, t')} / 2\pi V. \]

Finally, we can straightforwardly check by substitution that symmetry requirement (15a) is also met. The kernel we have just constructed can readily be applied when dealing with non-interacting scalar fields in homogeneous spacetimes, as we will come to discuss in section 5.

3. The kernel in the presence of a source

So far we have only examined the kernel for a free, non-interacting, quantum field. It is thus natural to turn to the interacting case which is particularly interesting for many physical situations. We will generalize the action in equation (16) and incorporate a spacetime-dependent source term \( J(x) \) coupled linearly to \( \phi(x) \). This particular type of interaction can model interactions with other scalar or fermionic fields, provided it is linear in one of the scalar fields. The action is given by

\[ S[\phi] = \int d^4x \sqrt{-g} \left( -\frac{1}{2} \partial_\mu \phi(x) \partial_\mu \phi(x) g^{\mu\nu} - \frac{1}{2} (m^2 + \xi R) \phi^2(x) + J(x) \phi(x) \right), \]

where, again, the time integral is performed over the finite interval from \( t' \) to \( t \) and the position integral is over all space. This action leads to the following equation of motion for the classical field:

\[ \Box \phi_{cl}(x) - (m^2 + \xi R) \phi_{cl}(x) = -J(x). \]

Fourier transforming and using the FLRW metric as before yields

\[ S[\phi_{cl} + \delta \phi] = S_0[\delta \phi] + \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} a^3(\tilde{t}) J_k(\tilde{t}) \phi_k(\tilde{t}), \]

analogously to equation (23). We split the quantum field as in (18) and require that the boundary conditions in the path integral in (14) are carried solely by the classical field. We thus arrive at

\[ S[\phi_{cl} + \delta \phi] = S_0[\delta \phi] + \frac{1}{2} \int d^3x \int_{t'}^t d\tilde{t} a^3(\tilde{t}) J_k(\tilde{t}) \phi_k(\tilde{t}). \]
The homogeneous solution of (41) is given by (25). Employing the Green’s function method and noting that only the homogeneous solution carries the boundary conditions, we find the following total solution:

$$\phi_k(\vec{r}) = \phi_k \frac{G_k(\vec{r}, \tau)}{G_k(\vec{t}, \tau)} + \phi_k \frac{G_k(t, \vec{t})}{G_k(t, \tau)} + S_k(\vec{r}),$$

(44)

where

$$S_k(\vec{r}) = \int_\tau^t d\tau Y_k(\vec{r}, \tau) J_k(\tau),$$

(45)

and where $Y_k(\vec{r}, \tau)$ is the appropriate Green’s function corresponding to (41),

$$Y_k(\vec{r}, \tau) = -\theta(\vec{r} - \tau) \frac{G_k(\vec{r}, \tau)}{W_k(\tau)} + \frac{G_k(\vec{r}, \tau)G_k(t, \tau)}{G_k(t, \tau)W_k(\tau)} - \theta(\tau - \vec{r}) \frac{G_k(\tau, \vec{r})}{W_k(\tau)} + \frac{G_k(\tau, \vec{r})G_k(t, \tau)}{G_k(t, \tau)W_k(\tau)}.$$  

(46)

Finally, we easily derive the symmetry relation $S_k(t) = S_k^*(t)$. Upon recalling the definition of the Wronskian, $W_k(t) = [\partial_t G_k(t, t')]|_{t'-t}$, we see that Green’s function (46) is, as expected, expressed solely in terms of the causal propagator. We proceed completely analogously by substituting expansion (44) into the action, equation (43), collecting all terms at each order, i.e., $\phi_k \phi_k^* \phi_k', \phi_k' \phi_k^* \phi_k$ and $\phi_k' \phi_k' \phi_k$ at quadratic order and $\phi_k, \phi_k', \phi_k^*$ and $\phi_k'$ as the linear contributions. The source contributes through the linear terms only and the quadratic ones remain unaffected. Furthermore, we can safely omit the terms at zeroth order in the fields, because we will incorporate those into the overall normalization. Hence the full result for the kernel reads

$$K(\phi, t; \phi', t') = \prod_k \mathcal{M}_k \exp \left[ -\frac{1}{V} \left( B(k, t, t') \phi_k \phi_k^* + C(k, t, t') \phi_k^* \phi_k' + \frac{1}{2} D(k, t, t') (\phi_k \phi_k^* + \phi_k^* \phi_k') + \frac{1}{2} E(k, t, t') \phi_k - \frac{1}{2} E^*(k, t, t') \phi_k^* ight) \right],$$

(47)

where $\mathcal{M}_k$ is again a normalization constant and where the $B$-, $C$- and $D$-functions are given by (30) and, finally, where

$$E(k, t, t') = -\frac{i}{2\hbar} \left[ a^3(t) \partial_t S_k(t) + \int_{\tau'}^t d\tau' a^3(\tau') J_k^*(\tau') \frac{G_k(\tau', t')}{G_k(t, \tau')} \right],$$

(48a)

$$F(k, t, t') = \frac{i}{2\hbar} \left[ a^3(t) \partial_t S_k(t') - \int_{\tau'}^t d\tau a^3(\tau) J_k^*(\tau) \frac{G_k(t, \tau)}{G_k(t', \tau')} \right].$$

(48b)

For a detailed derivation see [3]. The derivative $\partial_t S_k(t)$ should be interpreted as $\partial_t S_k(t)|_{t'=t}$. Since $E^*(k, t, t') = -E(-k, t, t')$, note that the contribution at order $\phi_k^*$ carries the opposite sign as compared to the contribution at order $\phi_k$ which mutatis mutandis holds for $F(k, t, t')$ and $F^*(k, t, t')$.

Let us now find the new normalization constant. The functional Schrödinger equation changes in comparison with (32) to

$$\left( i\hbar \partial_t - \int d^3 \mathbf{x} \left( -\frac{\hbar^2}{2a^3(t)} \frac{\delta^2}{\delta \phi(\mathbf{x})^2} + a^3(t) \left( \frac{1}{2} (m^2 + \xi R) \phi^2(\mathbf{x}) - J(\mathbf{x}) \phi(\mathbf{x}) \right) \right) K(\phi, t; \phi', t') = 0,$$

(49)
The position space form for the kernel (47) generalizes equation (33) to
\[
K(\phi, t; \phi', t') = M(t, t') \exp \left[ -\int d^3y d^3z [\phi(y)\phi(z)B(y, z) \right.
\]
\[+
\left. \phi'(y)\phi'(z)C(y, z) + \phi(y)\phi'(z)D(y, z) \right] \right] .
\]
(50)

Substitution into the functional Schrödinger equation (49) leads again to a number of equations at various orders in the fields \( \phi \) and \( \phi' \) that are indeed satisfied simultaneously. Writing \( M(t, t') = \int_k M_k(t, t') \), the zeroth-order equation in Fourier space reads
\[
\frac{i\hbar}{\partial t} \log M_k(t, t') - \frac{\hbar}{a^3(t)} \left\{ B(k, t, t') - \frac{1}{2V} |E(k, t, t')|^2 \right\} = 0.
\]
(51)

We can solve this equation straightforwardly by
\[
M_k(t, t') = M_{0,k} \sqrt{D(k, t, t')} \exp \left[ \frac{i\hbar}{2V} \int_{t'}^t d\tilde{t} \frac{|E(k, \tilde{t}, t')|^2}{a^3(\tilde{t})} \right],
\]
where \( M_{0,k} \) is again a time-independent constant. Note that the lower boundary of the integral is \( t' \) because our solution for the kernel is constructed such that it vanishes for times less than \( t' \).

Finally, \( M_{0,k} \) has to be fixed by condition (15) as before. Now, in the limit when \( \Delta t = t - t' \to 0 \) the kernel can easily be verified to be
\[
K(\phi, t; \phi', t) = \prod_k M_{0,k} \sqrt{\frac{ia^3(t)}{\hbar \Delta t}} \exp \left[ -\frac{a^3(t)}{2\hbar V \Delta t} \left( \phi_k - \phi'_k - \frac{\partial S_k(t)}{2} \Delta t \right) \right.
\]
\[\times \left. \left( \phi_k^* - \phi'_k^* + \frac{\partial S_k^*(t)}{2} \Delta t \right) + \frac{ia^3(t)}{8\hbar V} \partial S_k^*(t) \partial S_k(t) \right].
\]
(53)

The dominant terms in the exponent behave as \( 1/\Delta t \) as \( \Delta t \to 0 \) and, consequently, the terms involving the source all give a vanishing contribution in this limit. Equivalently, the shift of the delta-function induced by the source vanishes at the lower boundary. We conclude therefore that (53) indeed reduces to a representation of a delta-function correctly. The result for \( M_{0,k} \) is hence unchanged compared to the free case (38). Furthermore, note that the width of the Gaussian in the limit when \( \Delta t \to 0 \) behaves as \( \Delta \phi_0 \propto \Delta t \), which indicates an early time diffusive wave packet spreading in configuration space. Finally, it can easily be verified that the obtained solution satisfies the correct symmetry properties (15).

4. Causality in quantum mechanics

Let us now examine the causal structure of quantum field theory in the formalism developed above. In this section, we will prove that (a) the causal propagator (8) in position space vanishes when \( \|x - x'\| > |\eta - \eta'| \) in de Sitter space and (b) the same light cone structure is also present in the functional Schrödinger picture and can be inferred from the kernel we have constructed. Here \( \eta \) denotes conformal time defined by \( d\eta = dt/a(t) \). The clear geometrical interpretation of causality in position space cannot be easily transferred to Fourier space because a Fourier transformation is nonlocal: one cannot simply draw ‘light cones’ in Fourier space. A delicate cancellation occurs such that a superposition of Fourier modes cancel precisely outside past and future light cones.

Since FLRW spacetimes are conformal, their causality structure is most easily described in conformal coordinates, in which the light cones are simply \( \|x - x'\| = |\eta - \eta'| \).
In de Sitter space the scale factor $a(t) = e^{Ht}$ implies $a(\eta) = -1/(H\eta)$, $\eta < 0$ and $H$ is the Hubble parameter of de Sitter space. In de Sitter space in $D$ dimensions the Chernikov–Tagirov [11] scalar propagator reads [5, 12]

$$i\Delta_{ab}(x, x') = \frac{H^{D-2}}{(4\pi)^{D/2}} \Gamma \left( \frac{D}{2} - 1 \right) \frac{1}{2y_{ab}^2} + \frac{H^2}{16\pi^2} \sum_{n=0}^{\infty} \frac{\Gamma \left( \frac{1}{2} + n \right) \Gamma \left( \frac{1}{2} - n \right)}{\Gamma (\frac{1}{2} + v + n) \Gamma (\frac{1}{2} - v + n) y_{ab}}$$

$$\times \left( \frac{y_{ab}}{4} \right)^n \left[ \ln \left( \frac{y_{ab}}{4} \right) + \psi \left( \frac{3}{2} + v + n \right) + \psi \left( \frac{3}{2} - v + n \right) - \psi (1 + n) \right]$$

$$- \psi (2 + n) \right] + \mathcal{O}(D - 4), \quad (54),$$

where we have kept the $D$-dimensional form of the first (most singular) term that may lead to singular contributions in the limit when $D \to 4$. Note that $a$ and $b$ can be either $+$ or $-$, $v^2 = 9/4 - (m^2 + \xi R)/H^2$, $R = 12H^2$ and $\psi(z) = d[\ln \Gamma (z)]/dz$ as usual. Furthermore, $y_{ab}$ is given by

$$y_{ab} = a^2 H^2 \Delta x_{ab}^2. \quad (55)$$

The scalar function $y = y_{ab}\delta_{ab} = (1/4) \sin^2 (H\ell/2)$ is a simple function of the geodesic distance $\ell$ in de Sitter space. Since we are only interested in the two Wightman functions contributing to the causal propagator, we have

$$\Delta x_{+}^2 = - (\eta - \eta')^2 + r^2 \quad (56)$$

$$\Delta x_{-}^2 = - (\eta - \eta' + i\epsilon)^2 + r^2. \quad (57)$$

where $r = \|x - x'\|$. The causal propagator (8) thus follows as

$$\langle \Omega |[\hat{\phi}(x), \hat{\phi}(x')]|\Omega \rangle = i\Delta_{+,+}(x, x') - i\Delta_{-,+}(x, x') = \frac{H^{D-2}}{(4\pi)^{D/2}} \Gamma \left( \frac{D}{2} - 1 \right)$$

$$\times \left\{ \frac{1}{y_{+,+}^2} - \frac{1}{y_{-,+}^2} \right\} + \frac{H^2}{16\pi^2} \sum_{n=0}^{\infty} \frac{\Gamma \left( \frac{1}{2} + v + n \right) \Gamma \left( \frac{1}{2} - v + n \right)}{n \Gamma (\frac{1}{2} + v) \Gamma (\frac{1}{2} - v) y_{ab}}$$

$$\times \left( \frac{y_{ab}}{4} \right)^n \left[ \ln (y_{+,+}) - \ln (y_{-,+}) \right]. \quad (58)$$

Clearly, the first term represents the standard Hadamard singularity that every propagator contains. The two terms relevant to our calculation are the ones in curly parentheses. It can be shown that

$$\frac{1}{y_{+,+}^2} - \frac{1}{y_{-,+}^2} = \frac{1}{a^2 H^2} [-2\pi i \text{sgn}(\Delta \eta) \delta (r^2 - \Delta \eta^2)] + \mathcal{O}(D - 4) \quad (59)$$

$$\ln (y_{+,+}) - \ln (y_{-,+}) = 2\pi i [\theta (\Delta \eta - r) - \theta (\Delta \eta - r)], \quad (60)$$

where $\Delta \eta = \eta - \eta'$. While the Hadamard pole results in a singular contribution at the light cone $|\Delta \eta| = r$, the logarithmic cuts—which are a mathematical description for amplification of super-Hubble correlations occurring in accelerating spacetimes—are responsible for finite contributions within past and future light cones. Outside past and future light cones both contributions (59) and (60) vanish, as expected. Therefore, our causal propagator (58) also vanishes in these regions as it should. Although we performed the calculation in de Sitter spacetime, an analogous result should hold for more general spacetimes.
Now, we will show that our kernel analysis is consistent with the arguments put forward above. In the functional Schrödinger picture the causal propagator reads

\[
\langle \Omega | [\hat{\phi}(x, t_1), \hat{\phi}(x', t_2)] | \Omega \rangle = \int D\phi D\phi' \phi(x) \phi(x') \{ \Psi^*(\phi, t_1) \Psi(\phi', t_2) K(\phi, t_1; \phi', t_2) - \Psi(\phi, t_1) \Psi^*(\phi', t_2) K(\phi', t_2; \phi, t_1) \}.
\]

(61)

For simplicity, we consider the free kernel (29). The Gaussian vacuum wavefunctional (see [1, 2, 13]) is given by

\[
\Psi(\phi, t) = N(t) \exp \left[ - \int d^3y d^3z \phi(y) A(y, z, t) \phi(z) \right] = \prod_k N_k(t) \exp \left[ - \frac{1}{V} \{ \phi_k^* A_k(t) \phi_k \} \right],
\]

(62)

where \(N(t)\) is a normalization constant formally given by

\[
N(t) = N_0 \exp \left[ -i\hbar \int dt \int d^3x \frac{A(x, x, t)}{a^3(t)} \right],
\]

(63)

and where the \(A\)-function in Fourier space is given by

\[
A_k(t) = \frac{1}{2\hbar} a^3(t) \frac{\partial}{\partial t} [\log \{ \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) + \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) \}],
\]

(64)

where \(k = |\mathbf{k}|\) and where \(\mathbf{n}\) is a unit vector normal to an arbitrary plane through the origin in \(k\)-space. We see after substitution in the functional Schrödinger equation that \(\phi_k(t)\) and \(\phi_k^*(t)\) in fact obey (23). This solution differs slightly when compared to [1]. The form of (64) is dictated by the required invariance of \(A_k(t)\) under \(\mathbf{k} \rightarrow -\mathbf{k}\), and the difference is due to our definition of Fourier decomposition in terms of complex mode functions (22).

In principle, we could allow for an even more general argument of the logarithm, namely

\[
a_k \{ \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) + \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) \} + b_k \{ \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) + \hat{\theta}(\mathbf{k} \cdot \mathbf{n}) \phi_k(t) \}.\]

Then, we require \(|a_k|^2 - |b_k|^2 = 1\) and in order to preserve homogeneity \(\arg(a_k) = \arg(b_k)\). These states would correspond to the most general pure (minimum uncertainty) states with a ‘nonzero particle number’ \(|b_k|^2\).

Splitting \(A_k(t)\) into real and imaginary parts yields

\[
A_k(t) = \frac{1}{4\hbar |\phi_k(t)|^2} \left( 1 - i \frac{a^3(t) \partial}{\partial t} |\phi_k(t)|^2 \right).
\]

(65)

We can in fact perform the two functional integrals in (61) by introducing two additional sources in the exponent, varying with respect to these sources and setting them to zero subsequently,

\[
\langle \Omega | [\hat{\phi}(x, t_1), \hat{\phi}(x', t_2)] | \Omega \rangle = \frac{\delta}{\delta J(x)} \frac{\delta}{\delta J'(x')} \int D\phi D\phi' \{ \Psi^*(\phi, t_1) \Psi(\phi', t_2) K_{J, J'}(\phi, t_1; \phi', t_2) - \Psi(\phi, t_1) \Psi^*(\phi', t_2) K_{J, J'}(\phi', t_2; \phi, t_1) \} |_{J = J' = 0},
\]

(66)

where

\[
K_{J, J'}(\phi, t_1; \phi', t_2) = K(\phi, t_1; \phi', t_2) \exp \left[ - \int d^3z [J(z) \phi(z) + J'(z) \phi'(z)] \right].
\]

(67)

After some algebra we arrive at the following intermediate result, where the two Wightman functions can clearly be recognized:
\[ \langle \Omega | \Delta \phi(x, t_1), \phi(x', t_2) | \Omega \rangle = - \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{D(k, t_1, t_2)}{4(C(k, t_1, t_2) + A_k^*(t_2))} \right\} e^{ik \cdot (x - x')} \]

(68)

Note that both \( \Delta_{-+} \) and \( \Delta_{+-} \) are expressed in terms of causal Green’s functions and the initial state through \( A_k(t) \). The functional Schrödinger picture shows that the evolution of correlators can be fully expressed in terms of causal propagators and initial state only. This is to be contrasted to out-of-equilibrium field theories in the Heisenberg picture, where often one reads that in non-equilibrium problems there are two independent two-point functions: the spectral function (causal propagator, commutator) and the statistical propagator (anticommutator)\(^4\).

Employing the definitions of the occurring functions in terms of the fundamental solutions in equations (30) and (64), allows us to even further simplify this result to obtain

\[ \langle \Omega | \Delta \phi(x, t_1), \phi(x', t_2) | \Omega \rangle = \hbar \int \frac{d^3k}{(2\pi)^3} G_k(t_1, t_2) \text{sgn}(k \cdot \hat{n}) e^{ik \cdot (x - x')} \]

(69)

as it should be. We have used identity (26), which establishes the link with the Heisenberg picture fields. Note that the Wightman functions in (68) depend on the initial state through \( A_k(t) \) whereas the causal propagator does not. Hence, we have shown that the kernel although developed in Fourier space, preserves the causal structure in terms of light cones in position space, as depicted in figure 1.

Concluding, since the commutator is causal and the kernel is expressed solely in terms of this causal quantity, quantum mechanics in de Sitter spacetime is fully causal. This is in contrast to claims made, for example, in [15–21]. Apart from [15], the claims in the literature [16–21] are based on considering single-particle quantum mechanics, in contrast to the functional Schrödinger picture used in the present work. This means that causality of quantum mechanics can be fully appreciated only within the context of (relativistic) quantum field theory, and can lead to misleading results when viewed within the one-particle formulation of quantum mechanics.

If initial and final times are equal, the kernel (29) and (30) reduces to a delta-function, i.e., there is no propagation of the field. If both times differ, propagation is dictated by the commutator propagator and hence causality is preserved in general in quantum mechanics. Note finally that equations (6) and (7) support this statement. Although we have proved this consistency in de Sitter spacetime explicitly, we have no reason to believe that our result does not hold in FLRW and more general spacetimes. In fact, one could take the region in spacetime where the commutator (69) vanishes as the definition for light cones in general spacetimes.

5. Applications

To illustrate the applicability of the kernel, we will turn our attention to three explicit examples. We construct the kernel in both Minkowski and pure de Sitter spacetimes, where in the former

\(^4\) This comment is formal in nature and in fact we do not question the utility of considering separately the evolution of statistical and causal propagators [14].
case one can recognize the simple harmonic oscillator kernel. Finally, we will examine the evolution of the vacuum state for a non-interacting Hamiltonian in general FLRW spacetimes.

5.1. Example I: simple harmonic oscillator

Consider the simple harmonic oscillator toy model. Let us take the Minkowski metric, i.e., we set $a(t) = 1$ in the FLRW metric. In the minimally coupled case ($\xi = 0$), the equation of motion that the field modes $\phi_k(t)$ obey follows from (23) as

$$\left(\hat{q}^2 + \omega^2\right)\phi_k(t) = 0,$$

(70)

where $\omega^2 \equiv k^2 + m^2$. If we choose our fundamental solution of this equation of motion to be

$$\chi_k(t) = \frac{1}{\sqrt{2\omega}} e^{i\omega t} \theta(k \cdot \hat{n}) + \frac{1}{\sqrt{2\omega}} e^{-i\omega t} \theta(-k \cdot \hat{n}),$$

(71)

then this solution obeys the correct symmetry properties. Note that this choice is consistent with the Wronskian normalization condition (31). Again, we could have chosen an even more general solution of the form $\varphi_k(t) = a_k \chi_k(t) + b_k \chi_{-k}(t)$ and require $|a_k|^2 - |b_k|^2 = 1$. The Fourier transform of the causal propagator defined in (11) is hence given by

$$G_k(t, t') = \left[\sin(\omega(t-t'))\right] \text{sgn}(k \cdot \hat{n}).$$

(72)

The kernel for the simple harmonic oscillator follows as

$$K(\phi, t; \phi', t') = \prod_k \frac{\omega}{2\pi \hbar V \sin(\omega(t-t'))} \left[\exp\left[\frac{i\omega}{2\hbar V \sin(\omega(t-t'))}\right] \left\{\phi_k^*(\phi_{-k} + \phi_{-k}^*) \cos(\omega(t-t')) - 2\phi_k^* \phi_{-k}^*\right\}\right].$$

(73)

If we let $V \rightarrow 1$ this is indeed in agreement with standard quantum-mechanical results. It reproduces for example [22] where $m = 1$.

5.2. Example II: de Sitter universe

As a second example we consider the kernel for the inflationary de Sitter universe [9]. The solution of (23) in conformal time is thus given by

$$\phi_k(\eta) = a_k \chi_k(\eta) + b_k \chi_k(\eta),$$

(74)
where $\alpha_k$ and $\beta_k$ are two coefficients and

$$
X_k(\eta) = \frac{1}{a(\eta)} \sqrt{-\frac{\pi \eta}{4}} \left[ e^{i \frac{\eta}{4}} H_v^{(1)}(-k\eta) \theta(k \cdot \hat{n}) + e^{-i \frac{\eta}{4}} H_v^{(2)}(-k\eta) \theta(-k \cdot \hat{n}) \right],
$$

(75)

where $H_v^{(1)}$ and $H_v^{(2)}$ are the Hankel functions of the first and second kind, respectively, at order $\nu^2 = \frac{9}{4} - \frac{(m^2 + \xi R)}{H^2}$, see equation (39). The causal propagator now follows as

$$
G_k(\eta, \eta') = \frac{\pi}{4H(a(\eta)a(\eta'))^{3/2}} \left[ H_v^{(1)}(-k\eta) H_v^{(2)}(-k\eta') - H_v^{(2)}(-k\eta) H_v^{(1)}(-k\eta') \right] \text{sgn}(k \cdot \hat{n}).
$$

(76)

The causal propagator in turn fully determines our kernel (29).

5.3. Example III: the evolution of the vacuum state

As a final example, we can apply the kernel to an initial vacuum state for some non-interacting scalar fields. Thus, initially, we start with a vacuum state $|\Psi_1(\phi,t')\rangle$ and calculate its forward time evolution according to standard quantum-mechanical lore (1). We employ the functional Schrödinger picture as before and arrive at

$$
\Psi(\phi, t) = \int D\phi' K(\phi, t; \phi', t') \Psi(\phi', t').
$$

(77)

We can now conveniently exploit equation (29) for the kernel in the non-interacting case. The Gaussian vacuum wavefunctional is given by (62). In order to perform the functional integral in (77), we switch to Fourier space, complete the square and arrive at the following intermediate result:

$$
\Psi(\phi, t) = \prod_k \mathcal{M}_k(t, t') \mathcal{N}_k(t') \left( \frac{\pi V}{C(k, t, t') + A_k(t')} \right)^{1/2} \exp \left[ -\frac{1}{V} \left\{ B(k, t, t') - \frac{1}{4} \frac{D^2(k, t, t')}{C(k, t, t') + A_k(t')} \right\} \phi_k^* \right].
$$

(78)

Now we insert the definition of the causal propagator and the Wronskian in terms of the fundamental solutions. Indeed, one can show that the expression above reduces to the vacuum at time $t$,

$$
B(k, t, t') - \frac{1}{4} \frac{D^2(k, t, t')}{C(k, t, t') + A_k(t')} = A_k(t),
$$

(79)

and furthermore

$$
\mathcal{M}_k(t, t') \mathcal{N}_k(t') \left( \frac{\pi V}{C(k, t, t') + A_k(t')} \right)^{1/2} = \mathcal{N}_k(t),
$$

(80)

as desired.

6. Conclusion

We constructed the kernel for a scalar field in FLRW spacetimes in two cases: a free field (29) and one coupled to a source term (47). We showed that these kernels can be expressed solely in terms of the causal propagator and derivatives of the causal propagator. We have applied the
general formalism to three examples, the simple harmonic oscillator kernel (73), the kernel in de Sitter spacetime and the evolution of the Gaussian vacuum wavefunctional (78).

In our analysis, the causal structure of quantum field theory in the functional Schrödinger picture is manifest. We have shown that the causal propagator, given by the vacuum expectation value of the commutator, forms the essential function in terms of which the functional kernel is expressed. Therefore, our functional Schrödinger picture analysis reproduces the standard (Heisenberg picture) causality structure of FLRW spacetimes.

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