Aronszajn’s reproducing kernels and Feynman propagators

Construction of the Hilbert spaces of quantum mechanics

Pierre-Cyril Aubin-Frankowski

7 décembre 2017
Ecole polytechnique, Palaiseau

Abstract

This study shows how Aronszajn’s theory of reproducing kernels allows us to construct the Hilbert spaces of quantum theory. We show that the Feynman propagator is an example of a reproducing kernel under a boundedness condition. To every Lagrangian thus corresponds a Hilbert space that does not need to be postulated a priori. For the free non-relativistic particle, we justify mathematically the concept of spacetime granularity. Reproducing kernels allow for a functional, rather than distributional, description of the Hilbert spaces of quantum theory, including the Fock space.

Keywords: Reproducing kernel Hilbert spaces, Feynman path integrals, quantum theory Hilbert spaces

Résumé

Cette étude présente comment la théorie des noyaux reproduisants d’Aronszajn permet de construire les espaces de Hilbert de la physique quantique. Nous montrons que le propagateur de Feynman est un exemple de noyau reproduisant sous une condition de borne. A chaque lagrangien correspond ainsi un espace de Hilbert qu’il n’est pas nécessaire de postuler a priori. Dans le cas d’une particule libre non-relativiste, nous justifions mathématiquement le concept de granularité de l’espace-temps. Les noyaux reproduisants permettent une description fonctionnelle, et non distributionnelle, des espaces de la mécanique quantique, dont l’espace de Fock.

Mots clés : Espaces à noyaux reproduisants, intégrales de chemin de Feynman, espaces de Hilbert de la mécanique quantique

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

1Address: 14 rue Domat 75005 Paris, Phone number: 0142394480/0609821569, E-mail : pierre-cyril.aubin@polytechnique.edu
Introduction

This study stems from a questioning over the mathematical description of quantum physics, as the working space is most often confounded with $L^2(X)$, where $X$ is the space-time. The Hilbert space $L^2(X)$ is mathematically the completion of $\mathcal{D}(X)$, the space of $C^\infty(X)$-functions with compact support, for the standard hermitian scalar product $(\cdot, \cdot)_{L^2}$. The space $L^2(X)$ is not a space of functions, but a space of equivalence classes, which forbids to consider pointwise values for a given "function" $\psi \in L^2(X)$. The caveats expressed while presenting quantum physics are thus fully justified for $L^2(X)$, as well as for some Sobolev spaces. However, how can we explain the appearance of Dirac measures in this formalism? How do we justify going to a linear world through a correspondence principle? On what grounds could we build a functional theory, rather than distributional, of quantum mechanics?

We shall show in this study that the mathematical theory based on Aronszajn’s reproducing kernels (as it was introduced by Aronszajn in its seminal paper [1] or as presented by Laurent Schwartz in the chapter 9 of [2]) provides answers to these questions. This theory leads to manipulating functions rather than equivalence classes, while using Diracs, Hilbert spaces as well as Hilbert-Schmidt operators. The kernel class is a very general one, suited for semi-groups problems, for Fourier interpretations if invariance is involved, for differential geometry and shape spaces. Some classical examples of kernels include the Gaussian kernel, the Laplacian kernel, or the scalar product of $L^2$ itself. Green functions and the kernels often manipulated in physics rate among reproducing kernels. Mathematically, the theory of reproducing kernels is as deep as Hilbertian analysis since it inherits its properties. In practice, this theory offers a constructive approach to various problems, which bring us back to the construction of quantum mechanics through Feynman propagators without starting with its interpretation or with the associated partial differential equations. We refer to the very complete presentation of [3], in which one can find the state of the art of the theoretical aspects of reproducing kernels.

We will start by presenting the mathematical grounds of reproducing kernel Hilbert spaces. The second part will show how Feynman path integrals can be included in this frame. The third part will address some immediate conclusions related to group representation and quantum field theory.
1 Construction of reproducing kernel Hilbert spaces

Let \( X \) be a set with no particular structure (\( X \) is a finite or infinite collection of points, it is not necessarily a vector space). 'Space' will be intended as vector space in all that follows. By 'kernel' we mean a function that maps two elements of \( X \) to a value in a field (\( \mathbb{R} \) or \( \mathbb{C} \) for instance). Quantum mechanics only require to develop the complex case.

**Definition 1.1 (Positive definite kernel in \( \mathbb{C} \)).** A kernel \( K : X \times X \to \mathbb{C} \) is called positive definite if it verifies:

- the hermitian symmetry: \( \forall x, x' \in X, K(x,x') = \overline{K(x',x)} \) (its complex conjugate)
- the positivity condition:

\[
\forall (a_i)_{i=1..N} \in \mathbb{C}^N, (x_i)_{i=1..N} \in X^N, \sum_{i=1}^N \sum_{j=1}^N a_i \overline{a_j} K(x_i, x_j) \geq 0
\]

Such a kernel is a proto-scalar product over the set \( X \): that is symmetrical and positive definite but not necessarily bilinear. Any scalar product over a space \( X \) is as a matter of fact a positive definite kernel. If we consider the Gram matrix \( G \) associated with the \( (x_i)_{i=1..N} \) for the kernel \( K \), its positivity writes as:

\[
\forall (x_i)_{i=1..N} \in X^N, G := (K(x_i, x_j))_{i,j \leq N} \quad \forall a \in \mathbb{C}^N, a^\dagger Ga \geq 0
\]

Through the Gram matrix, the theory of reproducing kernels is intimately related to the theory of positive definite matrices. The notion of reproducing kernel is usually presented for real-valued kernels first, it also extends to vector-valued kernels.

**Examples of positive definite kernels with real values:**

- The Gaussian kernel over \( \mathbb{R}^n \), \( K(x, y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right) \), is positive definite.
- The Laplacian kernel over \( \mathbb{R}^n \), \( K(x, y) = \exp(-\lambda \|x - y\|_{\mathbb{R}^n}) \), is positive definite.
- The Cauchy kernel over \( \mathbb{R}^n \), \( K(x, y) = \frac{1}{1 + \frac{\|x-y\|^2}{\sigma^2}} \), is positive definite.
- The minimum kernel over \([0, 1]\), \( K(x, y) = \min(x, y) \), is positive definite.
- The maximum kernel over \([0, 1]\), \( K(x, y) = \max(x, y) \), is not positive definite.
- The kernel over \([-1, 1]\] defined by \( K(x, y) = \frac{1}{1-xy} \), is positive definite.

To show the positivity of a kernel, we use the property that the sum, the product, and the product by a positive scalar of positive definite kernels are positive definite.
**Definition 1.2 (reproducing kernel Hilbert space (RKHS)).** Let \((V, (\cdot, \cdot)_V)\) be a Hilbert space of complex-valued functions over \(X\). A kernel \(K : X \times X \to \mathbb{C}\) is a reproducing kernel of \(V\) if:

- \(V\) contains the function \(K_x : \{ X \to \mathbb{C} \}
  \begin{align*}
  y \in X &\mapsto K(x, y)
  \end{align*}
  \) when \(x\) ranges over \(X\),
- we have the *reproducing property*:
  \[
  \forall x \in X, \forall f \in V, f(x) = (f, K_x)_V
  \]

If such a reproducing kernel exists, the space \(V\) is called a *reproducing kernel Hilbert space.*

The functions \(K_x(\cdot)\) are related to the Dirac measures at \(x\) \((\delta_x)\). Furthermore, if the space \(V\) is a reproducing kernel Hilbert space, it has only one reproducing kernel. Reciprocally, a kernel can be reproducing for at most one space \(V\). We obviously have that:

\[
K(x, x) = (K_x, K_x)_V = \|K_x\|_V^2
\]

For the Gaussian kernel \(K(x, y) = \exp\left(-\frac{\|x-y\|_2^2}{2\sigma^2}\right)\) and \(X = \mathbb{R}^n\), we deduce that:

\[
\|K_x\|_V^2 = \exp\left(-\frac{\|x-x\|_2^2}{2\sigma^2}\right) = 1
\]

The Gaussian \(K_x(\cdot)\) are thus on the unit sphere of the space \(V_{\text{Gaussian}}\). Properties of this type are reminders of the interpretation of wave functions as probability amplitudes in quantum mechanics. We will make the relation explicit when defining the Feynman kernel.

**Lemma 1.1 (Description of \(V\)).** Let \(K_x : \{ X \to \mathbb{R} \}
  \begin{align*}
  y \in X &\mapsto K(x, y)
  \end{align*}
  \). The reproducing kernel Hilbert space \(V\), built from \(X\) and \(K\), is the completion for the kernel \(K\) of the space \(\text{Vect}(\{K_x\}_{x \in X})\), the space generated by the functions \(K_x\). The space \(\text{Vect}(\{K_x\}_{x \in X})\) is thus dense in \(V\) for the distance induced by the kernel.

The link between positive definite kernels and reproducing kernels is given by Aronszajn’s theorem (1950).

**Theorem 1.2 (Aronszajn).** A kernel \(K\) over \(X\) is positive definite if and only if there exists a space \(V \subset \mathbb{C}^X\) of complex-valued functions over \(X\) which is a Hilbert space and a function \(\Phi : X \to V\) such as:

\[
\forall x, x' \in X, K(x, x') = (\Phi(x), \Phi(x'))_V
\]
The reproducing kernel Hilbert space acts naturally as a functional ‘representation’ of the
set \( X \). The function \( \Phi \) embeds the set \( X \) (nonlinear by default) in a space \( V \), which constitutes the 'correspondence principle' of quantum physics.

Sometimes we would like to identify the space \( V \) associated with a given kernel (and later with the Lagrangian of a particle). However, identifying the Hilbert space of a reproducing kernel is as complex as identifying a Hilbert space from a differential form or from a Green kernel. There are however numerous techniques listed in 2.4 and 2.5 of \[3\] to facilitate this step, many kernels being very well known. For instance, the Gaussian kernel defines \( H^\infty_\sigma(\mathbb{R}^n) \) a completion of the Schwartz space, the Laplacian kernel defines the Sobolev space \( H^2_\lambda(\mathbb{R}^n) \) and the linear kernel \( (\cdot, \cdot)_{\mathbb{R}^n} \) the space of square integrable functions, related to \( L^2(\mathbb{R}^n) \).

The formulation of Aronszajn’s theorem nevertheless masks the true construction of kernels. The set \( X \) has no structure, to compute linear operations over it, it is necessary to embed it in the space of discrete measures \( F'(X) := \text{Vect}(\{\delta_x\}_{x \in X}) \), identifying each \( x \in X \) with \( \delta_x \) its Dirac measure in \( x \). The latter space does not have a topology yet.

**Definition 1.3.** We define by \( F'(X) \) the space of discrete measures over \( X \), i.e. \( \text{Vect}(\{\delta_x\}_{x \in X}) \) which is the algebraic dual of the space \( F(X) := \mathbb{C}^X \) of complex functions over \( X \). We endow \( F'(X) \) with the sesquilinear form \((\cdot, \cdot)_{V'}\):

\[
\forall N_0, N_1 \in \mathbb{N}^*, \forall ((x_i, a_i), (y_j, b_j)) \in (X \times \mathbb{C})^{N_0+N_1}, \left( \sum_{i=1}^{N_0} a_i \delta_{x_i} \sum_{j=1}^{N_1} b_j \delta_{y_j} \right)_{V'} := \sum_{i=1}^{N_0} \sum_{j=1}^{N_1} a_i \bar{b}_j K(x_i, y_j)
\]

**Lemma 1.4.** When the kernel \( K : X \times X \to \mathbb{C} \) is positive definite, \( (F'(X), (\cdot, \cdot)_{V'}) \) is a pre-hilbertian space which can be completed into a Hilbert space \( (V', (\cdot, \cdot)_{V'}) \). As \( F'(X) \) is embedded in \( V' \), we have the inverse relation for its dual space, the reproducing kernel Hilbert space: \( V \subset F(X) \).

**Proof:** This result stems from the definition of positive definiteness and classical results of duality in Hilbert spaces. The identity mapping from \( F'(X) \) to \( V' \) is indeed continuous with dense image in its completion (i.e. an embedding) as the measure space \( F'(X) \) is equipped with the weak topology. Therefore the dual space \( V \) of the completion is embedded as well in \( F(X) \) which is supplied with the pointwise convergence topology, .

Figure 1 recapitulates the construction of the reproducing kernel Hilbert space in a quantum mechanics context. It jointly presents the classical formulation through \( L^2(X) \) and the one through reproducing kernels. Figure 1 puts in vis-à-vis the Hilbert space \( L^2(X) \) and the space of functions \( V \) built over the kernel \( K \), which allows us to consider pointwise values of the 'function' \( \psi(\cdot) \in V \), the dual of the latter containing the Dirac measures. The role of the Schwartz space \( \mathcal{S}(X) \) and of its dual, the space \( \mathcal{S}'(X) \) of tempered distributions, is primordial in the canonical formulation which is related to the Fourier transform.
Figure 1: Summary of the various spaces appearing in the construction of the reproducing kernel Hilbert space, drawing a parallel between practice and theory in quantum mechanics.
2  The Feynman kernel

Which kernel should we choose to build a reproducing kernel Hilbert space? This is often a tricky question for the data analyst. In physics, when looking for a hermitian symmetry comparing two space-time positions, one may be inclined to think about Feynman propagators.

The set $X$ will be considered from now on as a subset of the space-time $\mathbb{R} \times \mathbb{R}^3$, the space of the four-position $x := (r, t) = \left( \frac{1}{2} \right)$. We suppose that we are given a Lagrangian $\mathcal{L}$ defined over the whole $\mathbb{R} \times \mathbb{R}^3$. The action along a trajectory $r(\cdot)$ going from $(r_0, t_0)$ to $(r_1, t_1)$ is defined as the integral of the Lagrangian along the trajectory. From now on we will write $x_0$ instead of $(r_0, t_0)$ to shorten the notations. The points will always belong to space-time.

For the propagator $K_{r_0,t_0}(r_1,t_1)$, we take Feynman’s definition as the sum of all the amplitudes (the complex exponential of the action $J$ defined by the Lagrangian $\mathcal{L}$) over all the trajectories $r(\cdot)$ with no restriction to the trajectories of least action. We shall denote by $J(x_0, x_1, r(\cdot)) := \int_{t_0}^{t_1} \mathcal{L}(r(s), \dot{r}(s), s) ds$ the action along a trajectory $r(\cdot)$ joining $x_0$ to $x_1$. We suppose given the existence of such a propagator, of finite complex value between two points in space-time.

2.1  Mathematical framework

Definition 2.1 (Feynman kernel). We define the propagator $K_{\text{Feyn}}$ (also known as the Feynman kernel) between two points $x_0 = (r_0, t_0)$ and $x_1 = (r_1, t_1)$ as the integral, normalized by a function $C(x_0, x_1)$, of all the trajectories $r(\cdot)$ going from $x_0$ to $x_1$.

$$K_{\text{Feyn}}(x_0, x_1) = \frac{1}{C(x_0, x_1)} \int_{r(t_0)=r_0}^{r(t_1)=r_1} \exp \left( \frac{i \cdot \text{sign}(t_1 - t_0) J(x_0, x_1, r(\cdot))}{\hbar} \right) dr(\cdot)$$

Lemma 2.1 (Product of propagators-Definition of the normalization). Let $x_0 := (t_0, r_0)$, $x_2 := (t_2, r_2)$ be two points and $t_1$ an in-between date such that $t_0 \leq t_1 \leq t_2$. We have that:

$$K_{\text{Feyn}}(x_0, x_2) = \int_{\mathbb{R}^3} dr_1 K_{\text{Feyn}}(x_0, x_1) K_{\text{Feyn}}(x_1, x_2)$$

Proof: By definition $J(x_0, x_2, r_{0,1} \diamond r_{1,2}(\cdot)) = J(x_0, x_1, r_{0,1}(\cdot)) + J(x_1, x_2, r_{1,2}(\cdot))$ where $r_{0,1} \diamond r_{1,2}(\cdot)$ is the concatenation of the paths $r_{0,1}(\cdot)$ going from $x_0$ to $x_1$ and $r_{1,2}(\cdot)$ going...
from \(x_1\) to \(x_2\). Every path joining \(x_0\) to \(x_2\) can be written like this for a well-chosen \(x_1\).

\[
K_{\text{Feyn}}(x_0, x_2) = \int_{t_0, t_1, t_2} \exp \left( \frac{i \cdot \text{sign}(t_2 - t_0) J(x_0, x_2, r_0, r_2)}{\hbar} \right) dr_0 dr_2
\]

\[
= \int dr_1 \int_{t_0, t_1, t_2} \exp \left( \frac{i \cdot J(x_0, x_2, r_0, r_2)}{\hbar} \right) dr_0 dr_2
\]

\[
= \int dr_1 \int_{t_0, t_1, t_2} \exp \left( \frac{i \cdot J(x_0, x_1, r_0, r_1)}{\hbar} \right) dr_0 dr_2 \cdot \int_{t_1, t_2} \exp \left( \frac{i \cdot J(x_1, x_2, r_1, r_2)}{\hbar} \right) dr_1 dr_2
\]

\[
= \int_{\mathbb{R}^3} dr_1 K_{\text{Feyn}}(x_0, x_1) K_{\text{Feyn}}(x_1, x_2)
\]

This integral is defined over the whole space but \(dr_1\) is a length element. \(K_{\text{Feyn}}(x_0, x_1)\) thus has a dimension with is the inverse of a length, in other words the dimension of a wave number \(k = 2\pi/L\). The normalization by \(C(x_0, x_1)\) was omitted above, as a matter of fact, the estimation of the normalizing coefficient actually stems from this multiplicative property (see for instance [4], p.166). We design \(C(\cdot, \cdot)\) based on the integral of the amplitudes, and thus depending on the Lagrangian. The function \(C(\cdot, \cdot)\) must verify:

\[
\forall t_0 \leq t_1 \leq t_2, \quad K_{\text{Feyn}}(x_0, x_2) C(x_0, x_2) = C(x_0, x_1) C(x_1, x_2) \int_{\mathbb{R}^3} dr_1 K_{\text{Feyn}}(x_0, x_1) K_{\text{Feyn}}(x_1, x_2)
\]

Under this condition, the lemma, which is a disguised definition of the normalization, is true.

**Preliminary remarks:**

- We do not know a priori the numerical value of \(K_{\text{Feyn}}(x_0, x_0) \in \mathbb{C}\).
- \(K_{\text{Feyn}}\) is hermitian, as a matter of fact, \(J(x_0, x_1, r(\cdot))\) is symmetrical in \(x\) but \(\text{sign}(t_1 - t_0)\) generates a negative sign in the exponential thus \(K_{\text{Feyn}}(x_0, x_1) = K_{\text{Feyn}}(x_1, x_0)\)

**Hypothesis:** Let \(A\) be a finite positive constant, we assume a hypothesis of homogeneity of space (which amounts to a normalization):

\[
\forall x \in X, \quad K_{\text{Feyn}}(x, x) = A \geq 0 \quad (1)
\]

We have a multiplicative property for any sequence \((x_i)_{i=2..N-1}\) belonging to a trajectory (not necessarily optimal) joining \(x_1\) to \(x_N\):

\[
\forall x \in X, \quad K_{\text{Feyn}}(x_1, x_n)/A = \prod_{i=1}^{n-1} (K_{\text{Feyn}}(x_i, x_{i+1})/A) \quad (2)
\]

The factor \(A\) appears in order to write a dimensionless equation. There is no integral here as we know that the particle was measured in \(x_i\), there is a 'wave function collapse'. Figure 2 illustrates this property.
Figure 2: Adding measures limits the possibilities, as the wave function collapse occurs at every point $x_i$.

**Lemma 2.2.** $K_{\text{Feyn}}$ is a positive definite kernel under a boundary condition where $l_P$ is a positive constant:

$$\max_{i=1 \ldots n} |K_{\text{Feyn}}(x_i, x_{i+1})| \leq \frac{2\pi}{l_P} \quad \text{and} \quad K_{\text{Feyn}}(x_i, x_i) \equiv A \geq 3 \cdot \frac{2\pi}{l_P}$$

**Proof:** $K_{\text{Feyn}}$ is hermitian. Let $S := \sum_{i=1}^{N} \sum_{j=1}^{N} a_i \overline{a_j} K(x_i, x_j)$, we must show its positivity for any sequence $(a_i)_{i \leq N} \in \mathbb{C}^N$.

The proof in the general case amounts to apply the multiplicity of $K_{\text{Feyn}}$ to recover the elementary pieces $K_{\text{Feyn}}(x_i, x_{i+1})$.

Let $(x_i)_{i=2 \ldots N-1}$ belonging to a trajectory joining $x_1$ to $x_N$. Thanks to equation (2), we may express the sum $S$ adequately based on the $K_{\text{Feyn}}(x_i, x_{i+1})$. Let $K_{\text{tr.sup.}}$ be the matrix of the first diagonal of the normalized Gram matrix and $\alpha$ the largest module of $K_{\text{Feyn}}(x_i, x_{i+1})$

$$K_{\text{tr.sup.}} := \begin{pmatrix}
0 & K_{\text{Feyn}}(x_1, x_2)/A & 0 & \ldots & 0 \\
0 & 0 & K_{\text{Feyn}}(x_2, x_3)/A & \ldots & 0 \\
0 & \ldots & \ldots & \ldots & 0 \\
0 & 0 & \ldots & 0 & \ldots & 0
\end{pmatrix}$$

$$\alpha := \max_{i=1 \ldots n} |K_{\text{Feyn}}(x_i, x_{i+1})|.$$
We rewrite the double sum $S$:
\[
S := \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K(x_i, x_j) = A \cdot a^\dagger \cdot \left( \text{Id} + \sum_{l=1}^{N} \left( (K_{\text{tr.sup.}})^l + (K_{\text{tr.sup.}}^\dagger)^l \right) \right) \cdot a
\]

We posit
\[
R := \sum_{l=1}^{N} \left( (K_{\text{tr.sup.}})^l + (K_{\text{tr.sup.}}^\dagger)^l \right)
\]

implying that $A \cdot a^\dagger (\text{Id} + R) a = S \geq 0 \iff \|a\|^2 \geq |a^\dagger Ra|$

We thus have to limit $a^\dagger Ra$:
\[
|a^\dagger Ra| \leq 2\|a\|^2 \cdot \sum_{l=1}^{N} (\alpha/A)^k = 2\alpha/A \cdot \|a\|^2 \cdot \frac{1 - (\alpha/A)^{N+1}}{1 - \alpha/A}
\]

Consequently:
\[
2\alpha \cdot \|a\|^2 \cdot \frac{1 - (\alpha/A)^{N+1}}{1 - \alpha/A} \leq A \cdot \|a\|^2 \Rightarrow S \geq 0
\]

We restrict ourselves to convergent sums for which $\alpha/A < 1$ and we take the limit in $N$:
\[
2\alpha \leq A \cdot (1 - \alpha/A) \Leftrightarrow \alpha \leq \frac{A}{3} =: k_p = \frac{2\pi}{l_p} \Rightarrow S \geq 0
\]

It thus suffices that:
\[
\max_{i=1,...,n} |K_{\text{Feyn}}(x_i, x_{i+1})| \leq \frac{2\pi}{l_p} = \frac{A}{3}.
\]

\[\blacksquare\]

**Remark:** This boundary condition is furthermore necessary and sufficient for an infinite number of measurements. If the sequence $(a_i)$ is taken constant equal to 1 and the $x_i$ such that $K_{\text{Feyn}}(x_i, x_{i+1}) = \alpha$, then:

\[
S = N \cdot A + \sum_{i \neq j} (\alpha/A)^{|i-j|} = N \cdot A + 2A \sum_{i=1}^{N} \sum_{l=1}^{N-i} (\alpha/A)^l = N \cdot A + 2\alpha \sum_{l=1}^{N} \left( \frac{1 - (\alpha/A)^{N+1-l}}{1 - \alpha/A} \right)
\]

\[
S \geq 0 \Leftrightarrow A \geq \frac{2\alpha}{1 - \alpha/A} \left( 1 - \frac{\alpha/A}{N} \cdot \left( \frac{1 - (\alpha/A)^{N+1}}{1 - \alpha/A} \right) \right) \xrightarrow{N \to +\infty} \frac{2\alpha}{1 - \alpha/A}
\]

**Remarks:**

- $V_{\text{Feyn}}$ is the Hilbert space of complex-valued functions which is the completion of the one generated by the wave functions $\psi_{r_0,t_0}(\cdot) := K_{\text{Feyn}}(x_0, \cdot)$ of a particle which has been measured in $x_0$ (which may be the point of its destructive measurement).

- $K_{\text{Feyn}}$ is a positive definite kernel thanks to a concatenation property of the trajectories.
2.2 Fundamental example: the free non-relativistic quantum particle

2.2.1 Detailed proof for \( N = 2 \)

Let us make explicit the value of \( S \) when \( N = 2 \) (corresponding to two measurements, at the beginning and the end of the experiment) and for a free non-relativistic quantum particle:

\[
S := a_1 \overline{a}_1 K_{Feyn}(x_1, x_1) + a_2 \overline{a}_2 K_{Feyn}(x_2, x_2) + a_1 \overline{a}_2 K_{Feyn}(x_1, x_2) + a_2 \overline{a}_1 K_{Feyn}(x_2, x_1)
\]

Le \( R \) be the cross term in \( S \).

\[
S = |a_1|^2 A + |a_2|^2 A + R \quad \text{R} := a_1 \overline{a}_2 K_{Feyn}(x_1, x_2) + a_2 \overline{a}_1 K_{Feyn}(x_2, x_1)
\]

For a free particle in classical mechanics, as reminded in [4], we have an explicit value for the propagator:

\[
K_{Feyn}(x_1, x_2) = \left( \frac{2 \pi \hbar (t_2 - t_1)}{m} \right)^{-1/2} \exp \left( \frac{im(x_2 - x_1)^2}{2\hbar(t_2 - t_1)} \right)
\]

We posit \( C_m := -\frac{m}{2\pi \hbar} \).

\[
K_{Feyn}(x_1, x_2) = \left( \frac{iC_m}{t_2 - t_1} \right)^{1/2} \exp \left( \frac{-i\pi C_m (x_2 - x_1)^2}{(t_2 - t_1)} \right)
\]

\[
= \sqrt{\frac{|C_m|}{|t_2 - t_1|}} \exp \left( \frac{i\pi \text{sign}(t_2 - t_1)}{4} \right) \exp \left( \frac{-i\pi C_m (x_2 - x_1)^2}{(t_2 - t_1)} \right)
\]

\[
R = 2|a_1||a_2| \sqrt{\frac{|C_m|}{|t_2 - t_1|}} \cos \left( \frac{\pi \text{sign}(t_2 - t_1)}{4} - \frac{\pi C_m (x_2 - x_1)^2}{(t_2 - t_1)} \right)
\]

In the worst case, the cosine term is equal to \(-1\). The kernel positivity thus amounts to require that:

\[
\forall a_1, a_2 \in \mathbb{C}, \forall t_1 \neq t_2, \ |a_1|^2 A + |a_2|^2 A - |a_1||a_2| \sqrt{\frac{|C_m|}{|t_2 - t_1|}} \geq 0
\]

We recognize an inequality of arithmetic and geometric means. The worst case corresponds to \( |a_1| = |a_2| \), \( A \) being defined by the hypothesis [1], it is thus necessary that:

\[
\forall t_1 \neq t_2, \ A \geq \sqrt{\frac{|C_m|}{|t_2 - t_1|}}
\]

It is necessary and sufficient for \( |t_2 - t_1| \) to be bounded below in order to have a finite constant \( A \). We have just shown that normalizing the propagator by a finite number is equivalent to postulating the existence of a positive lower bound over the durations between two measurements.
2.2.2 Discussion

Let's reformulate our conclusions in the case of a free particle for which:

$$\alpha := \max_{i=1\ldots n} |K_{Feyn}(x_i, x_{i+1})| = \sqrt{\frac{|C_m|}{\min_i |t_{i+1} - t_i|}}$$

where $$C_m := -\frac{m}{2\pi\hbar}$$

The upper bound over the modules of the elementary propagators is built on a lower bound

$$\delta t := \min_i |t_{i+1} - t_i|$$

over the duration between two consecutive measurements. We have not yet fixed the value of $$l_P$$ such that:

$$\sqrt{\frac{m}{\hbar \cdot \delta t}} \leq \frac{2\pi}{l_P}$$

We would like to choose a bound $$l_P$$ independent of the value $$m$$. As $$\delta t$$ is a lower bound over the durations between two measurements, lets give it the value of the Planck time

$$\sqrt{\frac{\hbar G}{c^3}}$$

the shortest duration known over which quantum theory applies. Our points $$x_i$$ are material points, the mass in $$x_i$$ cannot be superior to the Plank mass $$\sqrt{\frac{\hbar c}{G}}$$. We thus need $$l_P$$ to be smaller or equal to the Planck length $$\sqrt{\frac{\hbar G}{c^3}}$$.

However, we have that

$$\frac{A}{3} = k_p = \frac{2\pi}{l_P}$$

where $$\forall i, K_{Feyn}(x_i, x_i) \equiv A$$. Thus $$A$$ is huge, of the magnitude of $$10^{35}m^{-1}$$ which makes $$K_{Feyn}(x_i, \cdot)$$ a function "approaching" a Dirac measure. The hypothesis $$\alpha/A < 1$$ boiled down to require $$A$$ to be a physical limit over the values of propagators. Consequently normalizing $$K_{Feyn}$$ by a finite value did boil down to postulate a positive lower bound over the durations between two measurements and is related to considerations over Planck units.

2.2.3 Granularity of space-time and definition of the path integral

The conclusion of the example of a free non-relativistic quantum particle is that we had to postulate a positive lower bound over the durations between two consecutive measurements and thus a bound on distances of the same type between two points through the speed of light. However this changes the structure of the space-time subset $$X$$ which, rather than continuous like the four-position space ($$\mathbb{R} \times \mathbb{R}^3$$), becomes discrete. Mathematically this does not cause any problem in kernel theory as it is defined for any set $$X$$ (and not only over vector spaces). This granularity of space-time allows furthermore to define without difficulty the path integral, the existence of which we had postulated. Starting from $$x_0$$, the particle has to reach $$x_1$$ with a bounded speed through trajectories based on a discrete lattice. Therefore the number of trajectories going from $$x_0$$ to $$x_1$$ with bounded speed is not only countable but is even finite. The integral defining the Feynman kernel is in this context a finite sum and measure theory is not involved.
3 Reproducing kernels and quantum field theory

3.1 Group representations and reproducing kernels

We conclude with the question of group representation. We started our study with space-time (discrete or not), which was devoid of any topology. The Feynman kernel allows us to define an induced topology over space-time thanks to a topology over the dual. Nonetheless, even without a topology, it is possible to define algebraic properties of groups (such as the Poincaré group) acting over space-time. Algebraic and topological properties seem separated, we obviously need to associate the two in order to write theorems, but they are intrinsically of different nature (algebra and topology reunite in the definition of a unitary operator). The action of a group over space-time \(X\) is then embedded thanks to a representation theorem into a linear group of operators acting on the wave functions space \(V\).

We start with a few reminders of group representation theory, following the presentation in [5]. A representation \((\pi, V)\) of a topological group \(G\) acting on a set \(X\) in a topological vector space \(V\) is given by a morphism \(\pi : G \rightarrow GL(V)\) such that the mapping \(\{G \times V \rightarrow V\)
\[(g, v) \mapsto \pi(g) \cdot v\]
is continuous. If \(V\) is a Hilbert space, provided with a scalar product invariant under the action of \(G\), we say that \((\pi, V)\) is unitary. In the case of a reproducing kernel Hilbert space, it is necessary and sufficient for the kernel to be invariant under \(G\) (i.e. \(K(g \cdot x, g \cdot y) = K(x, y)\)) to retrieve a unitary representation of the form:

\[
\pi(\cdot) : \begin{cases}
G &\rightarrow GL(V) \\
g &\mapsto \begin{cases}
V &\rightarrow V \\
f(\cdot) &\mapsto f(g^{-1} \cdot)
\end{cases}
\end{cases}
\]

In our context, the space \(V\) is obviously the space \(V_{\text{Feyn}}\) built over the Feynman propagator. The transformation group \(G\) can be the Lorentz group or one of its sub-groups. If the propagator is invariant under their action (which is always the case for relativistic Lagrangians and the Lorentz group), these groups naturally become unitary groups acting on \(V_{\text{Feyn}}\). We may thus proceed with the presentation of the foundations of quantum field theory and of its groups, as written in the chapter 2 of [6].

3.2 Construction of the Fock space

Positive definite kernels have a very useful property: the sum, the product, and the product by a positive scalar of positive definite kernels are positive definite. This allows us to construct Hilbert spaces based on operations over kernels. We will limit ourselves to pointing out the emergence of tensor products of Hilbert spaces. There are nevertheless many other operations, such as the exterior product, as detailed in sections 2.2 and 2.3 of [3].

**Theorem (2.20 [3])**. Let \(X_1\) et \(X_2\) be two sets, let \(K_1 : X_1 \times X_1 \rightarrow \mathbb{C}\) and \(K_2 : X_2 \times X_2 \rightarrow \mathbb{C}\) be two definite positive kernel defined respectively over \(X_1\) and \(X_2\), and associated respectively with the reproducing kernel Hilbert spaces \(V_1\) and \(V_2\). The product of kernels
$K_1 \otimes K_2 : \left\{ \begin{array}{l}
(X_1 \times X_2) \times (X_1 \times X_2) \to \mathbb{C} \\
((x_1, x_2), (y_1, y_2)) \mapsto K_1(x_1, x_2)K_2(y_1, y_2)
\end{array} \right.$ is positive definite over the Cartesian product $X_1 \times X_2$ and the associated reproducing kernel Hilbert space is the tensor product $V_1 \otimes V_2$.

For two particles, the joint space-time $X_1 \times X_2$ is the Cartesian product of their respective space-times. The Hilbert space defined by their propagators is then the tensor product of their Hilbert spaces $V_1 \otimes V_2$. For the Feynman kernel this will lead to the definition of entanglement (i.e. that the tensor product $V_1^* \otimes V_2 = \mathcal{L}(V_1, V_2)$ is generated by and different to the space of linear operators of rank 1). However taking the product of propagators means summing their Lagrangians (thanks to the exponential morphism) along the joint trajectory (the cartesian product of the individual trajectories). We thus recover thanks to some fundamental properties of reproducing kernels the link between summing the Lagrangians and having tensor products of Hilbert spaces. This property is the origin of the Fock space.

**Conclusion**

In this study we have shown how reproducing kernel theory allow us to construct the Hilbert spaces of quantum mechanics (the spaces of the wave functions of one particle), which are different from the hermitian space $L_2$. We have followed a constructive approach through Feynman propagators and shown that the latter were reproducing kernels under a boundedness condition. We have finally related our work to the presentation by Steven Weinberg of the basis of quantum field theory while invoking only the notions of space-time, Lagrangians and actions along trajectories.

We had to postulate the existence of a finite value propagator, through a discrete version if necessary. As there are some Sobolev spaces $H^m(\mathbb{R}^n)$ that do not contain only functions (the ones for which $m \leq \frac{n}{2}$), Aronszajn’s reproducing kernels are based on another duality than the one of the ‘pivot space’ $L_2$. We would like to deepen the mathematical link between the two dualities. In physics, we would like to look for other consequences of the reproducing kernel framework on physical concepts.

I would like to thank deeply Jean-Louis Basdevant and Jean-Philippe Vert whose marvelous teachings inspired this manuscript.
References

[1] N. Aronszajn, Theory of Reproducing Kernels Transactions of the American Mathematical Society, 68, No. 3 (1950), pp.337-404

[2] L. Schwartz, Sous-espaces hilbertiens d’espaces vectoriels topologiques et noyaux associés (noyaux reproduisants), J. Analyse Math., 13 (1964), p. 115-256.

[3] S. Saitoh et Y. Sawano, Theory of Reproducing Kernels and Applications, Springer, Developments in Mathematics, 2016

[4] J-L. Basdevant, Les principes variationnels en physique, Vuibert, 2014

[5] D. Renard, Groupes et représentations, Ecole polytechnique, 2009

[6] S. Weinberg, The Quantum Theory of Fields, Vol 1 Foundations, Cambridge University Press, 1995