Boundary conditions: The path integral approach

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Abstract. The path integral approach to quantum mechanics requires a substantial generalisation to describe the dynamics of systems confined to bounded domains. Non-local boundary conditions can be introduced in Feynman’s approach by means of boundary amplitude distributions and complex phases to describe the quantum dynamics in terms of the classical trajectories. The different prescriptions involve only trajectories reaching the boundary and correspond to different choices of boundary conditions of selfadjoint extensions of the Hamiltonian. One dimensional particle dynamics is analysed in detail.

1. Introduction

The original approach to quantum mechanics due to Heisenberg and Schrödinger is based on the Hamiltonian formalism. Dirac and later Feynman introduced a Lagrangian approach. The Feynman’s path integral method was shown later to be equivalent to the traditional formulation for most of quantum mechanical systems [1, 2]. In field theory the method presents some advantages over Hamiltonian quantisation. The Lagrange formalism preserves relativistic covariance which makes the Feynman method very convenient to achieve the renormalization of field theories both in perturbative and non-perturbative approaches. In the Euclidean version [3] the functional integral formulation is a crucial ingredient for non-perturbative approaches to field theory and critical phenomena [4]. The equivalence of the functional integral formulation with the Hamiltonian pictures also holds for constrained systems like gauge theories and string theories.

However, for systems constrained to bounded domains Feynman’s approach becomes more intricate than the Hamiltonian operator approach and require a sophisticated implementation for generic types of boundary conditions compatible with Hamiltonian approach [5]. The analysis of this problem is the main goal of this paper. On the other hand the physics of quantum systems constrained to bounded domains is becoming very relevant not only for applications in condensed matter (quantum Hall effect, graphene, quantum wires, quantum dots, etc) but also in fundamental physics in fields like quantum gravity and string theory. In all these phenomena the role of boundary conditions is very important to describe a variety of new physical effects like anomalies [6, 7, 8] topology change [9] quantum holography [10, 11, 12], quantum gravity and AdS/CFT correspondence [13]. To some extent the relevance of boundaries in the description of fundamental physical phenomena has promoted the role of boundary phenomena from academic and phenomenological simplifications of complex physical systems to a higher status connected with very basic fundamental principles. The application of the path integral approach to those problems requires a radical generalisation of Feynman’s formalism.
2. Boundary conditions in quantum mechanics

Unitarity is the basic quantum principle which governs the dynamics of quantum systems confined in bounded domains. The analytical implementation of this condition in the selfadjoint character of the Hamiltonian operator encodes all the quantum subtleties associated to the unitarity principle and the dynamical behaviour at the boundary. The selfadjointness condition of the Hamiltonian imposes severe restrictions to the boundary conditions which are compatible with quantum mechanics.

The existence of a boundary generically enhances the genuine quantum aspects of the system. Well known examples of this enhancement are Young’s two slits experiments and the Aharonov-Bohm effect, which pointed out the relevance of boundary conditions in the quantum theory. Another examples of quantum physical phenomena which are intimately related to boundary conditions are the Casimir effect [14, 15] the role of edge states [16] and the quantisation of conductivity [17, 18] in the quantum Hall effect.

The quantum role of boundary conditions is very important for the behaviour of low energy levels. High energy levels are quite independent of boundary effects. Indeed, boundary effects play no role in the ultraviolet regime, whereas they are crucial for the infrared [19].

Let us consider a point-like particle moving on a bounded domain \( \Omega \) of \( \mathbb{R}^n \) with smooth oriented boundary \( \partial \Omega \). The Hamiltonian of the system can be constructed from the scalar Laplacian

\[
H = \frac{1}{2} \Delta = -\frac{1}{2} \sum_{i=1}^{n} \partial_i^2.
\]

This operator is symmetric on the domain of smooth wave functions with compact support on \( \Omega \). However, the restriction of the Laplacian operator to this domain is not selfadjoint, but it can be extended to larger domains of wave functions where it becomes selfadjoint. The extension, however, not unique.

The classification of selfadjoint extensions of the Hamiltonian can be characterised in terms of unitary operators between defect subspaces in the classical theory due to von Neumann [20, 21]. However, there is a more useful characterisation of these selfadjoint extensions in terms of constraint conditions on the boundary values of physical wave functions [22]. In this framework the set of self-adjoint extensions of the Hamiltonian is in one-to-one correspondence with the group of unitary operators of the Hilbert space \( L^2(\partial \Omega) \) of wave functions of the boundary \( \partial \Omega \) which are square integrable with respect to the Riemannian measure induced from the Euclidean metric of \( \mathbb{R}^n \).

Thus, any unitary operator \( U \) of the Hilbert space \( L^2(\partial \Omega) \) defines a selfadjoint quantum Hamiltonian \( \Delta^U \). And conversely, any selfadjoint extension of \( H \) is associated to one unitary operator \( U \) of this type [22]. The domain of the selfadjoint Hamiltonian governed by \( U \) is defined by the wave functions which satisfy the boundary condition

\[
\varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi}),
\]

where \( \varphi = \psi|_{\partial \Omega} \) is the boundary value of the wave function \( \psi \) and \( \dot{\varphi} \) its oriented normal derivative at the boundary \( \partial \Omega \). Through the above characterisation, the set of self-adjoint extensions of the Hamiltonian inherits the group structure of the group of unitary operators. For spaces of dimension higher than one the group of boundary conditions is an infinite dimensional group.

Since we shall focus on one-dimensional spaces two domains are of special interest: the compact interval \( \Omega = [0,1] \) and the half line \( \Omega = [0,\infty) \). Although the second domain is non-compact it will be useful to illustrate the main problems due to its simplicity. In the first case the set of boundary conditions is \( U(2) \) whereas for the half line it is \( U(1) \).
3. Boundary conditions in path integrals

In Feynman’s approach to quantum mechanics the dynamics is governed by an action principle similar to that which governs the classical dynamics. Whereas the classical dynamics is given, according to the variational action principle, by stationary trajectories of the classical action, the quantum dynamics is automatically implemented in the path integral formalism by the weight that the classical action provides for particle trajectories. In the Euclidean time formalism the evolution propagator for the free particle is given by the path integral

$$K_T(x, y) = e^{-TH}(x, y) = \int \delta x(t) \, e^{-\frac{1}{2} \int_0^T \dot{x}(t)^2 dt},$$

(3)

However, for particles evolving in a bounded domain the variational problem is not uniquely defined in classical mechanics. In order to have a deterministic evolution it becomes necessary to specify the evolution of the particles after reaching the boundary. A similar ambiguity problem arises in quantum mechanics.

The boundary imposes more severe constraints on the classical dynamics than in the quantum one. This is due to the point-like nature of the particle which requires that after reaching the boundary the individual particle has to reemerge back either at the same point or at a different point of the boundary. In pure classical mechanics the only freedom concerns where it reemerges back and the momentum it reemerges with. The emergence of the particle at a different point grants the possibility of folding and gluing the boundary of the domain giving rise to non-trivial topologies. In summary, the classical boundary conditions are given by two maps [23]: an isometry of the boundary $\alpha : \partial \Omega \to \partial \Omega$ and a positive density function $\rho : \partial \Omega \to \mathbb{R}^+$ which specify the change of position and normal component of momentum of the trajectory of the particle upon reaching the boundary. The isometry $\alpha$ encodes the possible geometry and topology generated by the folding of the boundary and the function $\rho$ is associated to the reflectivity (transparency or stickiness) properties of the boundary. However, the quantum boundary conditions have a larger set of possibilities described by a unitary group. In order to have a path integral description of all boundary conditions we need to incorporate some random behaviour for the trajectories reaching the boundary and complex phases for those trajectories. This is possible because the wave functions are complex and the evolution operator involves complex amplitudes. Although, is this way we are able to describe any type of unitary evolution in the bounded domain the method goes far beyond Feynman’s pure action approach.

The prescription is quite involved and proceeds by considering instead of the Euclidean time evolution propagator $K_T$ the resolvent operator $C_z$ of the Hamiltonian

$$C_z(x, y) = (z \mathbb{I} + H)^{-1}(x, y) = \int_0^\infty \frac{dT}{T} e^{-zT} K_T(x, y).$$

(4)

The Euclidean time propagator can be recovered from the resolvent by means of the following countour integral

$$K_T(x, y) = \frac{1}{2\pi i} \oint C_z(x, y)e^{zT} dz$$

(5)

along a contour which encloses the spectrum of $H$ on the real axis.

Boundary conditions can be easily implemented into the resolvent, whereas as we shall see that the implementation in the Euclidean time propagator is much harder. Let us consider a fixed boundary condition, e.g. the Neumann boundary conditions $U = \mathbb{I}$, and consider the corresponding Hamiltonian $H_0$ as a background selfadjoint operator. The selfadjoint extension of $H$ defined on the domain

$$i(\mathbb{I} + U)\varphi = (\mathbb{I} - U)\varphi$$

(6)
by the unitary operator $U$ has a resolvent given by Krein’s formula [24]

$$C_z^U(x, y) = C_z^0(x, y) - \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) R_z^U(w, w') C_z^0(w', y),$$

(7)

where $R_z^U$ is the operator of $L^2(\partial\Omega)$ defined by

$$R_z^U = ((I - U) C_z^0 - i(I + U))^{-1}(I - U).$$

(8)

A similar formula could be obtained choosing another boundary condition as background boundary condition instead of Neumann’s condition.

The inverse transform permits to recover a formula for the propagator kernel of the type

$$K_T(x, y) = K_T^0(x, y) - \frac{1}{2\pi i} \int dz e^{zT} \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) R_z^U(w, w') C_z^0(w', y).$$

(9)

It is easy to rewrite $K_T^0(x, y)$ as a path integral as in (3) restricting the trajectories to the interior of the domain $\Omega$ and counting twice the trajectories hitting the boundary $\partial\Omega$. However, in general, the kernel $K_T(x, y)$ cannot be rewritten in terms of a path integral. Only for a few boundary conditions the reduction can be achieved, but for generic boundary conditions the kernel $K_T(x, y)$ has to be considered as a genuine boundary condition kernel containing information about the boundary jumps amplitudes and phases associated to the different trajectories hitting the boundary. The complex structure of this kernel reduces the utility of the path integral approach and points out the behaviour of the boundary as a genuine quantum device. This behaviour can be explicitly pointed out by noticing that under certain boundary conditions the quantum evolution of a narrow wave packet is scattered backward by the boundary as a quite widespread wave packet emerging from all points of the boundary.

However, there are cases where this kernel adopts a simple form and the path integral approach can be formulated in very explicit way. In particular, for Dirichlet boundary conditions $U = -\mathbb{I}$,

$$R_z^U = (C_z^0)^{-1}$$

(10)

and

$$C_z^D(x, y) = C_z^0(x, y) - \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) (C_z^0)^{-1}(w, w') C_z^0(w', y),$$

(11)

which leads to a propagator kernel given by the path integral (3) but restricted to paths which do not reach the boundary $\partial\Omega$.

Further examples can be explicitly analysed for one-dimensional domains.

4. Particle in a half line

In order to illustrate the method let us consider for simplicity the unbounded domain $\Omega = [0, \infty]$. The set of selfadjoint extensions is parametrised by $U(1)$, i.e. the unitary operators of the form $U = e^{i\alpha}$. The corresponding boundary conditions are the mixed conditions

$$\varphi(0) = -\varphi'(0) = -\tan\frac{\alpha}{2}\varphi(0).$$

(12)

The resolvent of the corresponding selfadjoint extension can be obtained from the Krein formula (7) giving rise to

$$C_z^U(x, y) = \frac{1}{2\sqrt{2z}} e^{-\sqrt{2z}|x-y|} + \frac{1}{4z} \frac{2z - \sqrt{2z}\tan\frac{\alpha}{2}}{\tan\frac{\alpha}{2} + \sqrt{2z}} e^{-\sqrt{2z}(|x|+|y|)},$$

(13)
which in the two extreme cases $\alpha = 0$ (Neumann)

$$C_0^\alpha(x, y) = \frac{1}{2\sqrt{2\pi z}} e^{-\sqrt{2\pi z}|x-y|} + \frac{1}{2\sqrt{2\pi z}} e^{-\sqrt{2\pi z}(|x|+|y|)}$$

(14)

and $\alpha = \frac{\pi}{2}$ (Dirichlet)

$$C_0^{\pi/2}(x, y) = \frac{1}{2\sqrt{2\pi z}} e^{-\sqrt{2\pi z}|x-y|} - \frac{1}{2\sqrt{2\pi z}} e^{-\sqrt{2\pi z}(|x|+|y|)}$$

(15)

is reduced to very simple formulas. Notice that because

$$R_2^D = \sqrt{2\pi z}$$

the Dirichlet resolvent $C_0^{\pi/2}$ can be easily obtained from the Neumann resolvent $C_0^0$ from Krein’s formula (7).

The inverse Laplace transform gives the following formulas for the Euclidean evolution kernels with Neumann boundary conditions [25, 26]

$$K_N^T(x, y) = \frac{1}{\sqrt{2\pi T}} e^{-|x-y|^2/2T} + \frac{1}{\sqrt{2\pi T}} e^{-|x+y|^2/2T}$$

(17)

and Dirichlet boundary conditions

$$K_D^T(x, y) = \frac{1}{\sqrt{2\pi T}} e^{-|x-y|^2/2T} - \frac{1}{\sqrt{2\pi T}} e^{-|x+y|^2/2T},$$

(18)

which can be interpreted in terms of the path integral as a sum over paths which never reach the boundary [25, 26], whereas the Neumann kernel corresponds to double-counting the paths which hit the boundary 1. Notice that the terms depending on $x + y$, which appear in (17) (18) (14)and (15), break translation invariance due to the existence of finite boundaries of the interval.

5. Particle in an interval.

If the particle is confined in an interval $[0, 1]$ the set of selfadjoint extensions is parametrised by $U(2)$. Although the general theory can be developed on the same basis, we shall consider only few cases where the path integral approach is simplified.

i) Neumann boundary conditions $U = \mathbb{I}$, $\tilde{\varphi} = 0$.

The resolvent with Neumann boundary conditions at both ends of the interval is (see e.g. [27, 28])

$$C_N^\alpha(x, y) = \frac{1}{2\sqrt{2\pi z}} \left[ e^{-\sqrt{2\pi z}(x+y)} + \frac{e^{-\sqrt{2\pi z}(2-x-y)}}{1 - e^{-2\sqrt{2\pi z}}} + \frac{e^{-\sqrt{2\pi z}|x-y|}}{1 - e^{-2\sqrt{2\pi z}}} + \frac{e^{-\sqrt{2\pi z}(2|x+y|)}}{1 - e^{-2\sqrt{2\pi z}}} \right].$$

The Euclidean time propagator kernel

$$K_N^T(x, y) = \frac{1}{\sqrt{2\pi T}} \left[ \sum_{n=-\infty}^{\infty} e^{-(x-y+n)^2/2T} + \sum_{n=-\infty}^{\infty} e^{-(x+y+n)^2/2T} \right]$$

1 In the Euclidean approach the restrictions imposed on the paths for Neumann and Dirichlet boundary conditions are interchanged with respect to the boundary conditions in the Minkowski approach, where the Dirichlet problem is associated to an infinite totally reflecting wall.
corresponds to a path integral where the trajectories which hit the boundary are double weighted as in the half line case.

ii) Dirichlet boundary conditions \( U = -1, \varphi(0) = \varphi(1) = 0 \)

The resolvent with Dirichlet boundary conditions at both ends of the interval is

\[
C^D_z(x, y) = \frac{1}{2\sqrt{2\pi}} \left[ \frac{e^{-\sqrt{2\pi}|x-y|}}{1 - e^{-2\sqrt{2\pi}}} + \frac{e^{-\sqrt{2\pi}(2-|x-y|)}}{1 - e^{-2\sqrt{2\pi}}} - \frac{e^{-\sqrt{2\pi}(x+y)}}{1 - e^{-2\sqrt{2\pi}}} - \frac{e^{-\sqrt{2\pi}(2-x-y)}}{1 - e^{-2\sqrt{2\pi}}} \right].
\]

The associated propagator kernel

\[
K^D_T(x, y) = \frac{1}{\sqrt{2\pi T}} \sum_{n=-\infty}^{\infty} e^{-(x-y+m)^2/2T} - \sum_{n=-\infty}^{\infty} e^{-(x+y+m)^2/2T}
\]

corresponds to a path integral where the trajectories reaching the boundary have been removed.

iii) Periodic boundary conditions \( U = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), \( \varphi(0) = \varphi(1), \varphi'(0) = -\varphi'(1) \)

The resolvent

\[
C^P_z(x, y) = \frac{1}{2\sqrt{2\pi}} \left[ e^{-\sqrt{2\pi}|x-y|} + \frac{e^{-\sqrt{2\pi}(1-x+y)}}{1 - e^{-2\sqrt{2\pi}}} + \frac{e^{-\sqrt{2\pi}(1+x-y)}}{1 - e^{-2\sqrt{2\pi}}} \right]
\]

and the propagator kernel

\[
K^P_T(x, y) = \frac{1}{\sqrt{2\pi T}} \sum_{n=-\infty}^{\infty} e^{-(x-y+n)^2/2T}
\]

indicate that the corresponding path integral is performed over periodic trajectories which cross from one end of the interval to the other.

iv) Pseudo-periodic boundary conditions.

The selfadjoint Hamiltonian corresponding to the unitary operator

\[
U = \begin{pmatrix} 0 & e^{-i\epsilon} \\ e^{i\epsilon} & 0 \end{pmatrix}
\]

is defined in the domain satisfying the boundary conditions

\[
\varphi(1) = e^{i\epsilon}\varphi(0) \quad \varphi'(1) = e^{i\epsilon}\varphi'(0).
\]

The resolvent

\[
C^P_z(x, y) = \frac{e^{i\epsilon(y-x)}}{2\sqrt{2\pi}} \left[ e^{-\sqrt{2\pi}|x-y|} + \frac{e^{-\sqrt{2\pi}(1-x+y)}}{1 - e^{-2\sqrt{2\pi}}} e^{-i\epsilon} + \frac{e^{-\sqrt{2\pi}(1-y+x)}}{1 - e^{-2\sqrt{2\pi}}} e^{i\epsilon} \right]
\]

and propagator

\[
K^P_T(x, y) = \frac{1}{\sqrt{2\pi T}} \sum_{n=-\infty}^{\infty} e^{-(x-y+n)^2/2T+i\epsilon(n+x-y)}
\]

kernels correspond to a path integral over periodic trajectories which are weighted with and additional phase factor \( e^{i\epsilon} \) for everytime they cross the (periodic) boundary from left to right and \( e^{-i\epsilon} \) if they cross it in opposite direction.
The method of images also permits to use unconstrained path integrals to describe systems with non-trivial boundary conditions [29]. However, in the case higher dimensions the method is not useful in the presence of non symmetric boundaries and the path integral cannot be defined by a simple prescription as in the Feynman original formulation.

For some boundary conditions of one dimensional systems it is possible to use another method based on the path integral approach with simpler boundary conditions but with an additional singular potential in the Euclidean action [30]. Two interesting cases are the following.

v) Quasi-periodic boundary conditions.

The selfadjoint extension corresponding to the unitary operator

\[ U_{\alpha} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ \sin \alpha & -\cos \alpha \end{pmatrix} \]  

is defined in the domain of quasiperiodic wave functions

\[ \varphi(1) = \tan \frac{\alpha}{2} \varphi(0); \quad \varphi'(1) = \cotan \frac{\alpha}{2} \varphi'(0). \]  

In this case the resolvent, Euclidean time propagators and path integral can be identified with those of periodic boundary conditions with an extra potential term in the action corresponding to a \( \delta'(x) \) singular interaction.

vi) A circle with a defect point.

The Hamiltonian with boundary conditions corresponding to the unitary matrix

\[ U = \frac{1}{2 - ia} \begin{pmatrix} ia & 2 \\ 2 & ia \end{pmatrix} \]  

can be thought as equivalent to the Hamiltonian of a delta function \( a\delta(x) \) potential acting on a particle moving a circle with the usual periodic boundary conditions \( U = \sigma_1 \) [31, 32] The corresponding formulae for the propagator kernel can be also written in a compact way [32, 33].

However, the method is only restricted to similar cases and for generic boundary conditions a closed form expression is not available. In higher dimensions the number of boundary conditions for which the path integral method is useful to describe the quantum evolutions is even more limited.

6. Conclusions

In summary, it is possible to generalise the Feynman approach to describe the dynamics of quantum systems constrained to bounded domains. The boundary itself has to be considered from this point of view a genuine quantum device and transitions amplitudes are required to implement the effect of the boundary into the path integral approach. For some boundary conditions the modification of the path integral formula includes a phase factor or a boundary weight for the trajectories which reach the boundary. However, the method becomes not useful for generic boundary conditions because the prescription becomes very intricate. This fact is a consequence of the enhancement of genuine quantum effects by the presence of the boundary.

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