Quantum Boundary Conditions

and

Geometric Phases

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Mathematics is a part of Physics.
Physics is an experimental science,
a part of natural science.
Mathematics is the part of Physics
where experiments are cheap.

V.I. Arnol’d [1]
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Introduction

In this thesis we investigate the presence of a geometric phase in a quantum nonrelativistic system: a particle in a box with moving walls and given boundary conditions. So, if on the one hand, the main target is the calculation of the connection one form, according to the theory of geometric phases, on the other it is necessary to have a well-defined Hamiltonian, and so to classify all possible self-adjoint extensions of the Laplacian in one dimension.

In this spirit what follows has been divided into three main parts: the first chapter centered on the tools needed from the theory of geometric phases, the second one where we summarize the main results about self-adjoint extensions of symmetric operators based on the nature of some boundary conditions. In the third chapter, instead, chosen some particular boundary conditions, we prove the existence of a geometric phase associated to the system. The thesis ends with a couple of appendixes about topics which are largely used through the chapters. But, before delving into all this, we would like to give a brief introduction about the main ideas which have been developed and how they have been structured in this thesis.

As stated above, the first chapter deals with geometric phases and how they were discovered. We start with a review on the adiabatic theorem, which represents a fundamental tool in the transition between time-independent systems and time-dependent ones.

From the standard derivation of the theorem we move on to the geometrical interpretation given by Kato, which naturally leads to a profound understanding of the so-called Berry’s phase in terms of the (an)holonomy on some space.

As a matter of fact one considers an extremely slow evolution of a given system under the influence of some external parameters. A standard example is provided by a spin one-half particle in a cyclically evolving magnetic field; in this case the
parameter manifold is simply the sphere $S^2$, since a three dimensional unit vector, the magnetic field, can be parametrized by two polar angles.

The anholonomy, as we are going to discuss, represents “the failure of the physical situation to return completely to its original state upon a cycle of a parameter dependent system in parameter space” and is a peculiar feature of the geometry of the parameter space.

A classical example of (an)holonomy is provided by the parallel transport of a vector around a loop on a sphere: after a turn around the vector forms a nontrivial angle with the initial vector which is proportional to the solid angle subtended by the closed path on the sphere. Moreover this factor depends only on the geometry of the sphere. Another classical example is provided by Focault’s pendulum: a pendulum in circular motion on the Earth acquires an extra phase factor, the so-called Hannay’s angle, due to our planet’s rotation. A less trivial, but still classical example, is provided by a very interesting problem in geometrical mechanics: The falling cat problem. A cat dropped from rest with its feet pointing up will be able to rotate itself of 180° on its way down although its angular momentum is zero. The paradox is solved by recalling that a cat is not a rigid body, and is capable of using his muscular structure in order to change its shape. So our falling cat has the same initial and final shape, but in the midst it twists itself and is able to change its shape. In other words the shape of the cat is cyclically evolving in shape space, whose final result is a 180° rigid rotation in real space. The (an)holonomy in this case is the rotation of the cat in physical space. See Figure 1.

Let us return to the quantum mechanical world and the realm of quantum phases. Berry’s ideas were anticipated by S. Pancharatnam, in his investigation on the polarization states of light. The Indian physicist considered the problem of how to define the phase difference between two light waves in different states of polarization, and as later showed by Berry, he was basically introducing a notion of “distant parallelism” on the Poincaré sphere, whose points are used to represent polarization states.

But it was only in 1984 that M. Berry and B. Simon unveiled the geometrical structure of adiabatic evolution, and as we are going to show later on in chapter one, the cyclic adiabatic evolution of a quantum system defines a parallel transport on a suitable fibre bundle.
Figure 1: The falling cat problem.
Introduction

Figure 2: The Rosetta Stone which bridged the gap between the physical theory of gauge fields and the mathematical formulation of connections on principal fiber bundles.

This has to be considered a success of the “geometrization process” in physics. There is no doubt, in fact, that geometric structures arise quite naturally in the development of modern theoretical physics, especially in the case of gauge theories, which are supposed to describe all fundamental interactions. In 1975 [9] T.T. Wu and C.N. Yang understood that mathematicians and physicists had been independently studying the same subject but naming it differently. If on the one hand, the physicists were investigating the nature of fundamental interactions and understanding the role of gauge fields, on the other, instead, the mathematical theory of fiber bundles and connections on principal fiber bundles was being developed independently. Wu and Yang were aware of this situation so that in their paper they reported a Rosetta Stone between the two languages (Figure 2).

C.N. Yang was so impressed by the intertwist between the two approaches to drive to the house of Shiing-Shen Chern and here it is his fist-hand story [10]:

I said I found it amazing that gauge fields are exactly connections on fiber bundles, which the mathematicians developed without reference to the physical world. I added “this is both thrilling and puzzling, since you mathematicians dreamed up these concepts out of nowhere.” He immediately protested, “No, no. These concepts were not dreamed up. They were natural and real.”
It is in this natural context of geometrical interpretations that the Berry phase was eventually discovered; the standard derivation of this extra phase factor and its interpretation in terms of (an)holonomy in a principal fiber bundle will be deeply analyzed in chapter one.

Extraordinary experimental efforts have been made in order to detect geometric phases through various techniques and methodologies. Moreover, further improvements were made both from the theoretical perspective and from the experimental one showing how geometric phases naturally arise in different fields of quantum theories, and in particular in condensed matter physics where they have found their natural habitat. These will conclude chapter one and the geometric foundations of the problem.

Next we move on to chapter two and analyze the problem of determining self-adjoint extensions of symmetric operators. In the operatorial description of quantum mechanics self-adjoint operators are used to describe effectively observables on physical systems. In some cases, physical reasoning gives a formal expression for the Hamiltonian and other observables as operators on a particular realization of the Hilbert space such as $L^2(M, d\mu)$. Most physical operators are unbounded so we need to consider the domains where they are defined. Usually, one starts looking for some symmetric domain and tries to check whether it is essentially self-adjoint or not. In the negative case, then, one is forced to study various self-adjoint extensions. Moreover, in the spirit of the Stone theorem, self-adjoint operators can be interpreted as the infinitesimal generators of the admissible transformations on the Hilbert space of physical states. The choice of the “right” self-adjoint extension is usually guided by physical intuition.

In chapter two we are going to develop the theory of self-adjoint extensions of symmetric operators according to von Neumann’s theory of unbounded operators and to classify them with the help of deficiency subspaces. Since our final target is going to be the analysis of self-adjoint extensions of the Laplacian on an interval, which is a second order differential operator, we are going to focus our attention on boundary conditions and their involvement in the search of suitable extensions.

In the last few years there has been increasing interest on the topology of boundary conditions and their effects on the quantum mechanical description of physical systems [11][14]. Boundary conditions have proved to be useful in the investigation of different areas in physics, ranging from edge states in the Hall effect to quantum
gravity and string theory. Moreover, it is well known that the introduction of boundaries in some quantum systems gives rise to peculiar phenomena like the Casimir effect [15]. There is a subtle difference between quantum and classical boundary. Take for example a classical particle bouncing against a wall. The region on the boundary interested in the reflection of the particle is local, and only a small part of the wall is interested in the dynamics of the collision. In addition to that, the bouncing is described phenomenologically, that is in terms of the elastic properties of the material and so on. The analogous situation in quantum mechanics is slightly different, because the whole wall, that is the whole boundary, is interested in the description of the process. In quantum mechanics the boundary behaviour is encoded in the Hamiltonian and in the conservation of probability, in other words in unitarity. These assumptions are based on physical principles and are much more stringent than those in classical physics.

The use of boundary conditions is becoming more and more relevant in quantum gravity and string theory. For example no quadrupole and octupole components have been observed in the experimental investigation of the cosmic microwave background radiation, and this may be linked to some global property of the topology of the Universe. In addition, it is more and more plausible that spatial topology in quantum gravity cannot be a time-invariant property and that any eventual theory has to incorporate topology change as a peculiarity [11]. In fact the application of quantum mechanics to general relativity suggests that virtual processes at high energies may cause violent fluctuations in geometry. As a result, change in space-time topology may occur; but a topology change is nothing but a smooth change in boundary conditions in Hilbert space. In [11, 12] and then in [14] it is pointed out that topologically different boundary conditions which are consistent with unitarity correspond to different self-adjoint extensions of the Hamiltonian. All these extensions are interpolated through the space of possible unitary boundary conditions. (See Figure 3). Thus a quantum mechanical approach to topology change could even shed some light on the spacetime texture as well.

Self-adjoint extensions of symmetric operators can be investigated by analyzing some quadratic forms, known as boundary forms and their vanishing on some suitable domains. Throughout chapter two we are going to classify all self-adjoint extensions of the Laplacian on a fixed interval in terms of the vanishing of boundary
forms, and we are going to show their physical interpretations in terms of scattering of plane waves.

The technology involved with boundary forms has a flaw because its applicability is mainly restricted to the case of differential operators. Another approach to the problem is provided by boundary triples, described in chapter two, which can be seen as naturally arising from the boundary form technique but can be used in a far more general context. They can be considered as a powerful tool in this kind of problems.

At last we move on to chapter three, which is the core of this work. We take a particle in a one dimensional box with moving walls, and would like to prove the existence of a geometric phase in the case of a cyclic adiabatic evolution. First of all we need to specify the domain of definition of the Hamiltonian. Since the walls are not fixed the problem consists of a family of Hamiltonians defined over changing domains. This is already a complicated problem that needs to be well posed. Moreover, in light of chapter two, one needs to choose a particular family of self-adjoint extensions and hope for the phase to be there. Dirichlet boundary conditions do not provide a good starting point (since they do not provide non-trivial phases) so we decided to consider other extensions.
After having studied its spectral decomposition we are ready to compute the one-form connection associated to our problem and compute its circulation on a certain closed path in the parameter space. A technical problem shows up: the coefficients of the one-form need to be handled with care, since divergent contributions may arise from the boundary and a prescription on how to renormalize the result is indeed necessary.

If we consider different values of the parameter which label our boundary conditions, we can have associated spectral decomposition of different kind. In the previous discussion a non-degenerate spectrum was assumed, so that an Abelian phase was expected to be found. On the other hand there are some cases where the spectrum could be degenerate and one needs to consider the Wilczek-Zee phase, which is a natural non-abelian generalization of the Berry phase. With these considerations the curtains fall over chapter three.

The thesis ends with three appendixes: the first one is about Sobolev spaces and their usefulness in the study of extensions of the Laplacian; the second one, instead, is a quick review of some ideas about connections on principal fiber bundles, which are the main course of the present work. The last one provides some ideas on the link between the boundary form associated to the Laplacian and the Wronskian of an ordinary second order differential equation.
Chapter 1

Geometric Phases

For God’s sake, please give it up.

Fear it no less than the sensual passion, because it, too,
may take up all your time and deprive you of your health,
peice of mind and happiness.
(Farkas Bolyai\textsuperscript{1})

Out of nothing,
I have created a strange new universe.
(Janos Bolyai\textsuperscript{2})

1.1 Adiabatic Evolution

From the axioms of quantum mechanics we know that given a quantum system one can associate to it a self-adjoint operator, the Hamiltonian, which, among other things, determines the time-evolution of the system. In order to investigate how the system evolves in time one needs to solve the Schrödinger equation ($\hbar = 1$):

\[
    i\partial_t \psi(t) = H(t)\psi(t),
\]

\textsuperscript{1}A letter to his son János urging him to give up his work on non-Euclidean geometry
\textsuperscript{2}A reference to the creation of a non-Euclidean geometry
where $\psi(t)$ is some state, i.e. a unit vector in a Hilbert space, e.g. $L^2(\mathbb{R})$. The solutions of the Schrödinger equation in the time-independent case are well-known in literature [16, 17], while in the time-dependent one they need more care.

In the most general situations it is not possible to write down an explicit solution of (1.1), due to the operatorial nature of the Hamiltonian. However, sometimes we are interested in slowly-changing systems so that, in the so-called adiabatic approximation, one can give an approximate solution to the Schrödinger equation.

Adiabaticity plays a fundamental role in physics since it is at the borderline between statics and dynamics; in fact it keeps track of infinitely slow dynamical effects, so that it is no longer static but its evolution is extremely slow. Adiabatic evolution has, of course, its counterpart in classical mechanics [18] where one considers adiabatic invariants, which for time-dependent Hamiltonians are the objects closest to conserved quantities. The construction of such invariants, which approximate well-enough integrals of motion, can be accomplished as a result of the adiabatic approximation.

A first formulation of the adiabatic theorem was given by Born and Fock [19], although Kato’s seminal paper [20] represents a cornerstone in the geometrical interpretation of such a slow evolution.

A general formulation of the adiabatic problem is the following. Let $\tau > 0$ be a fixed constant representing the total time of the evolution and let us rescale the time coordinate $t \to s = t/\tau$, so that $s \in [0, 1]$, and the Schrödinger equation reads:

$$i\partial_s\psi_\tau(s) = \tau H(s)\psi_\tau(s). \quad (1.2)$$

We are now interested in what happens in the limit $\tau \to \infty$. There are several forms of the theorem, which all depend on the regularity properties of the given data, but share the same structure. Given, in fact, a suitable family $P(s)$ of spectral projections of $H(s)$, we suppose that the initial state $\psi_\tau(0) \in \text{Range}P(0)$, then for some $\gamma \geq 0$:

$$\text{dist} (\psi_\tau(s), \text{Range}P(s)) \leq o(\tau^\gamma). \quad (1.3)$$

In other words if we start the evolution in an eigenspace, then the dynamically evolved state can be approximated as much as we want by a state in the final evolved eigenspace.
One question may arise naturally: What is the meaning of a “slowly-varying” time evolution? Of course one needs to define a reference time-scale, so that the expression “fast” and “slow” are well-posed. If we start from an isolated eigenvalue in the spectrum, we can define an intrinsic temporal scale, and we can also estimate how good our approximation is. In the gapless case the theorem holds, as well, but since there is no characteristic time scale we cannot infer about the rate at which our approximation is reached. For some recent applications of adiabaticity in terms of shortcuts for scale invariant driving see the interesting paper [21].

In this chapter we follow the beautiful presentation of the topic given by Chruściński and Jamiolkowski [22].

1.2 The Born-Fock approximation

In 1928 [19] Born and Fock proved a version of the theorem for an Hamiltonian with a non degenerate and discrete spectrum so that we can write:

\[ H(t) u_n(t) = E_n(t) u_n(t) \]  

with the choice of normalized eigenvectors. To avoid technicalities we consider a finite dimensional Hilbert space, e.g. \( \mathcal{H} = \mathbb{C}^l, l \in \mathbb{N} \). This assumption forces a discrete spectrum, and in addition we suppose, for simplicity, that it is not degenerate. If we start at \( t = 0 \) with \( \psi(0) = u_n(0) \), then the state at a later time \( t \) will be given by the following sum:

\[ \psi(t) = \sum_{m=1}^{l} c_m(t) \exp \left( -i \int_{0}^{t} E_m(s) ds \right) u_m(t). \]  

From now on the superscript index in the summation, denoting the dimension of the Hilbert space will not be reported. In the last expression we have factorized the dynamical phase factor so that, if we take (1.5) and plug it into the Schrödinger equation we find a differential equation for the Fourier coefficients \( c_m(t) \):

\[ \frac{d}{dt} c_m(t) = -c_m(t) \langle u_m(t), \dot{u}_m(t) \rangle + \]

\[ - \sum_{k \neq m} c_k(t) \langle u_m(t), \dot{u}_k(t) \rangle \exp \left[ -i \int_{0}^{t} (E_k(s) - E_m(s)) ds \right]. \]
Before discussing the adiabatic approximation we need another relation. Take equation (1.4), differentiate it in time and consider its scalar product with a generic eigenstate $u_m$:

$$\langle u_m, \dot{u}_k \rangle = \frac{1}{E_k - E_m} \left\langle u_m, \dot{H} u_k \right\rangle \quad k \neq m,$$

(1.7)

where time-dependence is understood. It is fundamental to remark one aspect of adiabatic evolution. Firstly, time evolution of the systems we are going to study will be implemented by some external parameters, (see for instance section 2.4), for example the well known case of a spin one-half particle into a slowly varying magnetic field, whose intensity is kept constant. In the analysis of adiabatic evolution there are two temporal scales which need to be taken into account. The first one, $\tau$, is the temporal scale associated to the time evolution of the parameters, or, in other words, it tells us how rapidly the Hamiltonian varies with time. In the above example, it corresponds to the period of rotation of the magnetic field. Moreover, there is an intrinsic time scale, which is related to the difference between two close energy levels (see Figure (1.1)) and it is proportional to the intensity of the magnetic field, or more generally to $\|H\|$, and consequently to the eigenvalues of the Hamiltonian. The idea of adiabatic evolution is the following: we let the magnetic field vary so slowly ($\tau$ very large) that no transition between energy levels can occur, or alternatively we increase the difference between the energy levels and let $B$ vary at a given pace. Physically, in fact, what really matters is the ratio...
between the two time scales. Adiabaticity, then, means that the external time-
dependent parameters are not that fast to provoke a jump between close energy
levels during time evolution. In light of the previous discussion, let us consider
the sum over \( k \) different from \( m \) in (1.6), and try to find a sufficient condition
such that the adiabatic approximation holds. If we assume that all quantities that
appear in that sum, which are expected to be slowly varying, are constant in time
and if the system is in the state \( n \) at \( t = 0 \), we can set \( c_k = \delta_{kn} \) so that the sum
in the right-hand side of equation (1.6) becomes:

\[
\frac{1}{E_n - E_m} \left\langle u_m, \dot{H} u_n \right\rangle e^{-i(E_n - E_m)t} \quad m \neq n,
\]

which integrated reads:

\[
\frac{i}{(E_n - E_m)^2} \left\langle u_m, \dot{H} u_n \right\rangle \left( e^{-i(E_n - E_m)t} - 1 \right) \quad m \neq n.
\]

Then, a sufficient condition for the adiabatic approximation to hold is:

\[
\left| \frac{1}{(E_n - E_m)^2} \left\langle u_m, \dot{H} u_n \right\rangle \right| \ll 1.
\]

If we use the scaled temporal coordinate as defined in (1.2) and set \( \dot{H} \equiv H'(s) \),
then we get the following:

\[
\frac{1}{\tau} \left| \frac{1}{(E_n - E_m)^2} \left\langle u_m, H' u_n \right\rangle \right| \ll 1,
\]

which represent the sufficient condition we require in order to neglect the sum in
(1.6). This means, for example, that the system is changing over such a large
period of time \( \tau \) that the change in \( H \) referred to the period of oscillation between
two neighbouring levels is small compared to the energy involved in the transition.

In the adiabatic limit, then, equation (1.6) reduces to:

\[
\dot{c}_m(t) = -c_m(t) \left\langle u_m(t), \dot{u}_m(t) \right\rangle,
\]

with the initial condition \( c_m(0) = \delta_{n,m} \). Solving equation (1.12) and plugging the
result into (1.5) we find that:

\[
\psi(t) = c_n(t) \exp \left( -i \int_0^t E_n(s) ds \right) u_n(t),
\]
where:

\[ c_n(t) = \exp(i \phi_n(t)), \]  
\[ \dot{\phi}_n(t) = i \langle u_n(t), \dot{u}_n(t) \rangle. \]  

(1.14) (1.15)

For fifty years the contribution of this additional phase \( \phi_n \) was ignored by the physics community and believed to be unphysical, since it could have been neglected through a gauge transformation of the basis eigenvectors. Indeed if we perform a gauge transformation

\[ u_n(t) \rightarrow u'_n(t) = e^{i \lambda_n(t)} u_n(t), \lambda_n : \mathbb{R} \rightarrow \mathbb{R}, \]  

(1.16)

then, equation (1.4) will hold for the transformed states as well. Using the gauge freedom, we could have chosen the states:

\[ \tilde{u}_n(t) = e^{i \phi_n(t)} u_n(t), \]  

(1.17)

for which the Born-Fock gauge condition holds:

\[ \langle \tilde{u}_n, \frac{d}{dt} \tilde{u}_n \rangle = 0, \]  

(1.18)

and the state in (1.13) can be re written as:

\[ \psi(t) = \exp \left( -i \int_0^t E_m(s) ds \right) \tilde{u}_n(t), \]  

(1.19)

so that no extra contribution seems to appear. There are some cases when the latter machinery fails and it turned out that an extra purely geometrical phase is indeed needed. This extra contribution is linked to the geometrical properties of the quantum evolution.

### 1.3 Kato’s interpretation of Adiabaticity

In his seminal paper of 1950 [20], Kato introduces a new strategy of attack to adiabaticity. This new technique has a purely geometric flavour, and shows, once more, how powerful is the hybridization of analytical techniques along with geometrical ones. Kato introduces a fictitious unitary evolution, which is exactly
known, together with the unitary evolution generated by the system Hamiltonian, and proves that their actions on an initial state is the same in the adiabatic limit. Moreover the strong hypotheses of discrete and non-degenerate spectrum are relaxed, and the theorem, in Kato’s formulation, holds when we focus on an isolated eigenvalue whose associated projections have finite-rank. Let us go back to (1.2), where $\tau$ is determined by the speed of change of the Hamiltonian. Then Kato builds up a unitary operator for the adiabatic evolution, which maps $\text{Ran}P(0)$ onto $\text{Ran}P(s)$:

$$P(s) = U_{AD}(s)P(0)U_{AD}^{-1}(s),$$

(1.20)

and introduces the following Hamiltonian:

$$H_{\text{Kato}}(s) = \frac{i}{\tau}[\partial_s P(s), P(s)],$$

(1.21)

so that the adiabatic evolution operator determined by the Kato equation:

$$i\partial_s U_{AD}(s) = \tau H_{\text{Kato}}(s)U_{AD}(s)$$

(1.22)

satisfies the so-called intertwining condition (1.20). It is important to remark that by building up a unitary adiabatic evolution operator we are giving a prescription on how to parallel transport vectors in the Hilbert space of physical states. Of course, this procedure is not, in general, uniquely determined. Equation (1.20) is only telling us that a vector in $\text{Ran}P(0)$ is being unitarily mapped into a vector in $\text{Ran}P(s)$. If we think naively in terms of Euclidean spaces this is easily understood.
Given two vectors in a three-dimensional space there are infinitely many ways of rotating one into the other, but, once the generator of rotations has been fixed, we lose the arbitrariness of the choice, since we have given a prescription on how to effectively rotate the vector. Analogously in our case there are infinitely many ways to implement equation (1.20), but once the generator associated to the unitary operator is fixed we have decided how to make a realization of (1.20). For example both $H_{\text{Kato}}$ and $H_{\text{Kato}} + P f P$, where $f$ is some function, implement equation (1.20), though representing two different realizations of it.

Then, the adiabatic theorem states that (see Figure 1.2):

$$\|(U(s) - U_{\text{AD}}(s))P(0)\| \leq o(\tau^{-1}).$$

(1.23)

Kato’s discovery of the underlying geometrical structure of adiabatic evolution can help us understand the mutual interplay between adiabaticity and geometry. The key needed to unlock geometric phases from their cage is given by the following fact: the time dependence of the Hamiltonian (which is the crux of the adiabatic approximation) is given by the dynamics of some external parameters, whose domain may not be a linear space or a flat affine space but a much more intricated and interesting set: a differentiable manifold. In other words we are translating time evolution of a system into a path on some manifold.

To be more concrete if we consider a spin 1/2 particle into a varying magnetic field, of fixed intensity, then we can consider the sphere $S^2$ as the parameter manifold, since we have the freedom of choosing a space orientation for the magnetic field, that is to say two angles. It is well known from differential geometry that $S^2$ is a compact manifold, that needs at least to charts in order to be completely determined. Moreover, its curvature is non-trivial, though constant, which implies that if we take a tangent vector lying on its surface and let it run over a closed path lying entirely on the sphere, we obtain in general a different vector from the starting one. Instead, if we take a closed path on the affine plane and use the rigid parallel translations, which are naturally defined on an affine space, then after a turn around the vector will go back to its original position (Figure 1.3).

This fact is a fundamental and well-known ingredient in gauge theories and in general relativity, and shows the necessity, even in the context of nonrelativistic quantum mechanics, of a geometrical formulation of the theory [23]. Then, one should not be surprised that one of the first discoveries in the field of geometrical
phases was made exactly on a system similar to that described above, where one of the simplest non-trivial manifold is taken into account.

Let $\mathcal{M}$ be a manifold of dimension $n$ where external parameters are settled in, so that we have a family of parameter-dependent Hamiltonians:

$$x \in \mathcal{M} \rightarrow H(x).$$  \hfill (1.24)

We denote with $P(x)$ a finite-rank projection onto some part of the spectrum separated by the rest of it by a gap.

We build up a trivial vector bundle (for further details see Appendix B): $\mathcal{H} \times \mathcal{M}$ and project out the sub-bundle, whose fibers are the ranges of $P(x) \forall x \in \mathcal{M}$, and we call it spectral bundle:

$$\mathcal{H}_P := \bigcup_{x \in \mathcal{M}} F_x,$$  \hfill (1.25)

$$F_x = \text{Ran}P(x).$$  \hfill (1.26)

If we start from an initial state $\psi(0) \in \text{Ran}P(0)$ its adiabatic evolution, given by $H_{\text{Kato}}$, forces it to be in $\text{Ran}P(s)$ at any other time in the evolution, or in other words:

$$P^\perp(s)\psi(s) = (\mathbb{I} - P(s))\psi(s) = 0.$$  \hfill (1.27)
Considering, then, explicitly equation (1.22) we find that:

$$\partial_s \psi(s) = P^\perp(s)(\partial_s P(s))\psi(s),$$

that is $\partial_s \psi \in \text{Ran} P^\perp \iff P\partial_s \psi = 0$. So we can build a vanishing local 1-form in the parameter space:

$$0 = Pd\psi = P \sum_{k=1}^{n} \frac{\partial}{\partial x^k} \psi dx^k.$$  

(1.29)

Clearly this form is local, since it depends on the chosen chart, which in general does not cover the whole manifold, and most importantly it is vector valued. We have, thus, defined a parallel-transport rule on our fiber bundle $\mathcal{H}_P$, or equivalently a covariant derivative:

$$\nabla := Pd.$$  

(1.30)

The operator defined in (1.30) is linear, satisfies the Leibniz rule:

$$\nabla f \psi = (df) \psi + f \nabla \psi, \quad \forall f \in C^\infty(\mathcal{M}), \quad \forall \psi \in \mathcal{H}_P,$$

(1.31)

which can be easily proved using the definition in (1.30).

What is really astonishing is that the adiabatic evolution, realized by $U_{AD}$, $(\nabla \psi = 0)$ defines a parallel transport over the fiber bundle $\mathcal{H}_P$ along a path in $\mathcal{M}$.

### 1.4 Berry’s Phase: A standard derivation

In this paragraph we are going to derive the explicit structure of the Berry phase and we are going to unveil the intertwist between the geometry of the parameter space and quantum phases.

We start with a curve $C$ in the parameter space $\mathcal{M}$:

$$t \rightarrow x_t \in \mathcal{M}$$  

(1.32)

and consider a family of parameter dependent Hamiltonians defined over the parameter space. We suppose that $H(x)$ admits a purely discrete spectrum over the whole $\mathcal{M}$:

$$H(x)u_n(x) = E_n(x)u_n(x), \quad \langle u_n(x), u_m(x) \rangle = \delta_{n,m} \quad \forall x \in \mathcal{M}.$$  

(1.33)
Moreover, we require that the map
\[ x \in \mathcal{M} \rightarrow u_n(x) \in \mathcal{H} \quad (1.34) \]
be single-valued, at least locally on a patch of the manifold. Notice that the
eigenvectors in (1.33) are not uniquely determined since one could perform the
gauge transformation:
\[ u_n(x) \rightarrow \tilde{u}_n(x) = e^{i\alpha_n(x)}u_n(x), \quad (1.35) \]
\[ \alpha_n : \mathcal{M} \rightarrow \mathbb{R}, \quad (1.36) \]
leaving equation (1.33) unaltered. We, now, focus our attention on the \( n \)-th
eigenspace, assume it is not degenerate and apply the adiabatic approximation.
As in the previous paragraph we consider the rank-one projection \( P_n(x) \) and build
up a fiber in \( x \):
\[ \mathcal{H}_n(x) = \text{Ran} P_n(x) = \{ \alpha u_n(x) : \alpha \in \mathbb{C} \}. \quad (1.37) \]
Next we investigate the dynamical evolution and consider the restriction of the
family of Hamiltonians in (1.33) to the chosen path, so that time-dependence will
be implemented by the following composition:
\[ t \rightarrow x_t \in \mathcal{M} \rightarrow H(x_t). \quad (1.38) \]
Suppose we start with a vector \( \psi(0) = u_n(x_0) \) and let it evolve adiabatically, so
that for every \( t \) we can approximate the true evolved state with a state in the \( n \)-th
eigenspace:
\[ \psi(t) \in \mathcal{H}_n(x_t). \quad (1.39) \]
If we consider a cyclic evolution of parameters, that is to say \( \mathcal{C} \) a closed path on
\( \mathcal{M} \), then after a turn around the state \( \psi(T) \) still belongs to \( \mathcal{H}_n(x_0) \) but it may
differ from \( \psi(0) \) by a phase factor:
\[ \psi(T) = e^{i\gamma} \psi(0). \quad (1.40) \]
Naively one could think that this phase \( \gamma \) is solely determined by the dynamical
evolution of the system, that is:
\[ \gamma \propto \int_0^T E_n(t)dt, \quad (1.41) \]
but, as Berry discovered in 1984 [7], although earlier anticipations can be found in Pancharatnam [5], there exists an extra purely geometrical contribution depending only on the properties of the manifold and on the chosen path. From the adiabatic approximation (equation (1.13)) we can write:

\[ \psi(t) = \exp \left( -i \int_0^T E_n(\tau) \, d\tau \right) e^{i\phi_n(t)} u_n(x_t), \]  

(1.42)

where from (1.14):

\[ \dot{\phi}_n = i \langle u_n, du_n \rangle. \]  

(1.43)

We now define the following one-form:

\[ A^{(n)} := i \langle u_n, du_n \rangle, \]  

(1.44)

which, in local coordinates, can be rewritten as:

\[ A^{(n)} = A_k^{(n)} dx^k; \]  

\[ A_k^{(n)} := i \langle u_n, \partial_k u_n \rangle. \]  

(1.45)

(1.46)

Since \( \langle u_n, du_n \rangle \) is purely imaginary, the form defined in (1.44) can be recast as:

\[ A^{(n)} = - \text{Im} \langle u_n, du_n \rangle. \]  

(1.47)

Once defined the 1-form above, we can solve equation (1.43) integrating it over the path \( C \), so that the geometrical contribution, known as the \textit{Berry phase} is given by:

\[ \gamma_n(C) := \phi_n(T) = \oint_C A^{(n)}. \]  

(1.48)

The total phase shift \( \gamma \) can be explicitly split into a dynamical and a geometrical part:

\[ \gamma = - \int_0^T E_n(\tau) d\tau + \gamma_n(C). \]  

(1.49)

A short remark is needed: in the present thesis we have decided to set \( \hbar = 1 \), so that it does not explicitly appear in any of the calculations performed. It is important, however, to observe that \( \hbar \) would appear in the dynamical phase, but not in the geometrical phase. This is a sign of the fact that \( \gamma_n(C) \) is independent of the chosen evolution, but it is rather an intrinsic geometrical property, as proved by [24, 25].
From the Stokes theorem (Figure 1.4) we can transform the circulation of $A^{(n)}$ into a flux integral:

$$\gamma_n(C) = \int_{\Sigma} F^{(n)},$$

(1.50)

where $\Sigma$ is a surface whose boundary $\partial \Sigma$ is exactly the closed curve $C$ and $F^{(n)}$ is given by the exterior differential of $A^{(n)}$:

$$F^{(n)} = dA^{(n)} = -\text{Im} \left( du_n \wedge du_n \right).$$

(1.51)

In a local coordinate chart the above tensor can be recast into the following expression:

$$F_{ij}^{(n)} = \frac{1}{2} F_{ij}^{(n)} \, dx^i \wedge dx^j,$$

(1.52)

$$F_{ij}^{(n)} = - \text{Im} \left( \langle \partial_i u_n, \partial_j u_n \rangle - \langle \partial_j u_n, \partial_i u_n \rangle \right).$$

(1.53)

Under a gauge transformation (1.35) the one-form $A^{(n)}$ transforms like a gauge potential of electrodynamics:

$$A^{(n)} \rightarrow A'^{(n)} = A^{(n)} - d\alpha_n,$$

(1.54)
while:
\[ F'(n) = F(n), \]  
(1.55)
due to the identity \( d^2\alpha_n = 0. \)

Equation (1.55) shows that \( F(n) \) is a gauge-invariant quantity, as well as the Berry phase \( \gamma_n(C) \) due to equation (1.50).

Again, in analogy with classical electrodynamics the 2-form \( F(n) \) plays the role of the magnetic field, whose flux (in our case the Berry phase), is invariant under gauge transformations. This analogy is extremely fruitful since the above derivation can be understood in terms of connections over a principle fiber bundle, which is a powerful tool in gauge theories (for further details see Appendix B).

### 1.5 Simon and his great synthesis

In 1983 B. Simon \[8\] unveiled the geometrical structure underlying the derivation of Berry’s phase. We report his comment:

“The purpose here is first to advertise what Berry calls a “remarkable and rather mysterious result”, but more basically to try to take the mystery out of it by realizing that \( \gamma \) is an integral of a curvature so that Berry’s phenomenon is essentially that of holonomy which is becoming quite familiar to theoretical physicists.”

Simon’s comment is enlightening and provides and elegant interpretation of Berry’s phase in the framework of gauge theories, or in more mathematical terms, in the framework of connections on principal fiber bundles. In section (1.3) we showed how adiabatic evolution could be interpreted as a purely geometrical one, so that now we are able to look at this result from a wider perspective.

Let us explicitly build the \( n \)-th spectral bundle. We take as base space the manifold of the external parameters and as the fiber at a point \( x \) the \( n \)-th eigenspace of \( H(x) \). If we suppose that \( E_n(x) \) is nondegenerate and restrict ourselves only to normalized vectors then the fiber at \( x \) is:

\[ F_x = \{ e^{i\alpha(x)} u_n(x) : \alpha \in \mathbb{R} \} \simeq U(1). \]  
(1.56)
Next we consider the total space as:

\[ P = \bigcup_{x \in \mathcal{M}} F_x, \]  

so that the triple \((P, \mathcal{M}, U(1))\) is a \(U(1)\) principal bundle. As we are now going to prove there exists a natural connection on \((P, \mathcal{M}, U(1))\) related to the Hilbert space inner product: we define (in a natural way) a horizontal vector \(|h\rangle\), a vector which is orthogonal (in the Hilbert space sense) to the fiber \(F_x\):

\[ \langle u_n(x), h \rangle = 0. \]  

Such a connection is usually referred to as the Berry-Simon connection.

In order to understand the physical meaning of the horizontal lift defined by (1.58), we take a path \(C\) in \(\mathcal{M}\), \(t \rightarrow x_t\), and consider its horizontal lift \(t \rightarrow \psi(t)\) according to (1.58), that is:

\[ \langle u_n(x_t), \dot{\psi}(t) \rangle = 0. \]  

The latter can be reformulated in terms of the external differential acting on the parameter space, that is:

\[ \langle u_n, d\psi \rangle = 0, \]  

or equivalently:

\[ P_n d\psi = 0, \]  

If \(u_n(x_t)\) is in the Born-Fock gauge (1.18), studied in section 1.2, then the curve:

\[ t \rightarrow u_n(x_t), \]  

defines uniquely a horizontal lift of the curve \(C \subset \mathcal{M}\). Viceversa, if, for every curve in \(\mathcal{M}\), the corresponding eigenvector \(u_n(x_t)\) defines a parallel transport of \(u_n\), then a family \(u_n(x)\) is in the Born-Fock gauge. Thus we have proved a deep correlation between the physical intuition of adiabatic evolution and the mathematical concept of parallel transport with respect to the Berry-Simon connection.

Moreover, from the general theory of connections on a principal fiber bundle it is known (see Appendix B) that a connection can be defined either by a horizontal distribution or by a local Lie-algebra-valued one-form. If we consider a local section
Chapter 1. Geometric Phases

Figure 1.5: The horizontal lift $\tilde{C}$ of a closed path $C$ is not usually closed. The difference between the two ends can be accounted by the holonomy on the fibre, denoted by $\gamma_n(C)$.

of the $n$-th spectral bundle:

$$x \in \mathcal{M} \rightarrow u_n(x),$$

then a local connection form (in a fixed gauge for the states $u_n$ is given by a $u(1)$ one form:

$$iA^{(n)} = -\langle u_n, du_n \rangle,$$

which differs by a factor $i$ from the Berry potential. Thus the Berry phase, which we can associate to a curve $C$ is an element of the holonomy group of the Berry-Simon connection (see Figure 1.5).

1.6 Non-Abelian Phases

In 1984 [26] Frank Wilczek and Anthony Zee generalized the Berry phase derivation to the case of degenerate spectra, discovering the so-called non-Abelian Wilczek-Zee phase factor.

In the previous paragraph we started from the non-degeneracy hypothesis of the $n$-th eigenvalue. Let us now relax this request and suppose that the $n$-th eigenvalue
is $N$-times degenerate, that is:

$$H(x)\psi_{n a}(x) = E_n(x)\psi_{n a}(x), \quad a = 1, 2, ..., N. \quad (1.65)$$

This means that the $n$-th eigenspace is $N$ dimensional:

$$\mathcal{H}_n(x) = \left\{ \sum_{a=1}^{N} c_a \psi_{n a} : c_a \in \mathbb{C} \right\}. \quad (1.66)$$

As in the non-degenerate case we choose normalized vectors, that is:

$$\langle \psi_{n a}, \psi_{n b} \rangle = \delta_{a b}, \quad (1.67)$$

and express the non-uniqueness of the choice with the following transformation:

$$\psi_{n a}(x) \rightarrow \psi'_{n a}(x) = \sum_{b=1}^{N} U_{a b}(x) \psi_{n b}(x). \quad (1.68)$$

Then, we move on to an adiabatic evolution of $\psi(t)$ and consider a closed curve in the parameter space:

$$t \in [0, T] \rightarrow x_t \in \mathcal{M}, \quad (1.69)$$

such that $x_0 = x_T$. From the adiabatic theorem (equation (1.3)), if we start with a state $\psi(0) \in \mathcal{H}_n(x_0)$ and let it evolve adiabatically we are going to end up in the $n$-th eigenspace: $\psi(T) \in \mathcal{H}_n(x_T) = \mathcal{H}_n(x_0)$. In the nondegenerate case the initial and final state could differ only by a phase, that is a $U(1)$ transformation, here, instead, due to the degeneracy, they could be obtained one from the other through a unitary matrix $V \in U(N)$, that is:

$$\psi(T) = V \psi(0). \quad (1.70)$$

For the sake of definiteness let us suppose that $\psi(0) = \psi_{n a}$, for some fixed $a$ in $\{1, ..., N\}$. In the adiabatic approximation, then, the evolved state can be written as:

$$\psi(t) = \exp \left( -i \int_0^t E_n(s) \, ds \right) \sum_{b=1}^{N} U_{a b}^{(n)}(t) \psi_{n b}(x_t), \quad (1.71)$$
with $U^{(n)}$ an $N \times N$ unitary matrix. Plugging the latter expression into the Schrödinger equation we find:

$$\left( \left( U^{(n)} \right)^{-1} \dot{U}^{(n)} \right)_{ab} = -\langle \psi_{n,a}, \dot{\psi}_{n,b} \rangle.$$  \hfill (1.72)

If we define the following one-form (known as Wilczek-Zee potential): 

$$A_{ab}^{(n)} := i\langle \psi_{nb}, d\psi_{na} \rangle,$$ \hfill (1.73)

then, the unitary matrix $V$ we are looking for can be factorized into:

$$V = V_{\text{dyn}}V_{\text{geo}}.$$  \hfill (1.74)

The dynamical contribution is a trivial one:

$$V_{\text{dyn}} = \exp \left( -i \int_0^T E_n(s) \, ds \right) \mathbb{I}_N,$$ \hfill (1.75)

while the geometrical one, the so called geometric Wilczek-Zee factor, is expressed in terms of a path-ordered integral:

$$V_{\text{geo}} = U^{(n)}(T) = P \exp \left( i \oint_C A^{(n)} \right).$$ \hfill (1.76)

It is useful to remark that $A^{(n)}$ is a Hermitian matrix, and that for $N = 1$, we go back to the Abelian case of the Berry phase, showing how the Wilckzek-Zee factor is a direct generalization of the former’s work.

In the Abelian case we found a striking correspondence between the one-form connection $A^{(n)}$ and the electromagnetic gauge potential. For the non-Abelian case, we do expect some links between Yang-Mills theories \cite{27}, that is non-Abelian gauge theories, and the one-form connection in (1.73).

With this end in view we now try to interpret the Wilczek-Zee phase factor as an holonomy element on a suitable fiber bundle. We start building up a spectral bundle $E^{(n)}$, which is going to be an associated bundle to a principal fiber bundle:

$$E^{(n)} = \bigcup_{x \in \mathcal{M}} \mathcal{H}_n(x),$$ \hfill (1.77)
whose typical fiber is \( F = \mathbb{C}^N \). It is easy to show that this bundle is an associated vector bundle to the \( U(N) \) principal bundle. In fact, once we have fixed \( N \) orthonormal vectors \( \phi_1, \ldots, \phi_N \in H_n(x) \), we can define a fibre:

\[
F^{(n)}_x := \left\{ \sum_b U_{ab} \phi_b : U \in U(N) \right\} \simeq U(N),
\]

and build up a principal fiber bundle over \( \mathcal{M} \):

\[
P^{(n)} := \bigcup_{x \in \mathcal{M}} F^{(n)}_x.
\]

Let us now take a curve \( C \) in \( \mathcal{M} \) and consider its horizontal lift on \( E^{(n)} \). We say that \( \phi_a(t) \) is an horizontal lift with respect to a Wilczek-Zee connection if:

\[
\langle \psi_{nb}, d\phi_a \rangle = 0, \quad \forall a, b \in 1, \ldots, N,
\]

or equivalently:

\[
P_a d\phi_a = 0, \quad \forall a \in 1, \ldots, N.
\]

We can generalize the Born-Fock gauge to the non-Abelian case and find that it corresponds to a parallel transport operation with respect to the Wilczek-Zee connection. Most importantly we would like to show how \( A^{(n)} \) transforms under a gauge transformation like (1.68):

\[
A^{(n)}_{ab}' = i \langle \psi_{nb}', d\psi_{na}' \rangle = (UAU^* + i (dUU^*))_{ab}.
\]

The latter equation shows that \( A^{(n)} \) transforms as a gauge potential of a Yang-Mills theory, so that a degenerate spectrum has led us naturally to a non-Abelian gauge theory, where \( N \) is determined by the degeneracy degree.

The corresponding gauge field can be formulated in terms of \( A^{(n)} \) in the usual way:

\[
F^{(n)} = dA^{(n)} - iA^{(n)} \wedge A^{(n)},
\]

whose local components are:

\[
(F^{(n)}_{kl})_{ab} = \partial_k (A^{(n)}_{lb})_{ab} - \partial_l (A^{(n)}_{kb})_{ab} - i[A^{(n)}_k, A^{(n)}_l]_{ab},
\]

\[
(A^{(n)}_k)_{ab} = i \langle \psi_{nb}, \partial_k \psi_{na} \rangle.
\]
In the end we observe that $\mathcal{F}^{(n)}$ is a 2-form with values in the Lie algebra $\mathfrak{u}(N)$, so that it is clear that $V_{\text{geo}}$ represents an holonomy of the Wilczek-Zee connection.

### 1.7 The Physics of Quantum Phases

Berry’s discovery unveiled some properties of quantum mechanics, which had been neglected for a very long time. Although, Dirac himself [28], and others, e.g. Aharonov and Bohm [29] had studied the problem of topological phases, the geometry of the adiabatic evolution had not been completely understood before Berry. Today, we are also aware that adiabatic evolution is just a technical tool, since geometric phases can arise in general cyclic evolution as shown in the work of Aharonov and Anandan [24], and Samuel and Bhandari [25].

In the present section we would like to discuss a particular experiment, done by T. Bitter and D. Dubber in 1987 [30], which showed incontrovertibly the existence of the Berry phase in a spin system under the influence of a cycling magnetic field.

The paradigm of geometric phases is provided by a spin one-half particle in a slowly varying magnetic field, which plays the role of the external environment. The experiment we would like to discuss involves the measurement of the polarization of a beam of neutrons after the interaction with an helical magnetic field. The resulting shift, if any, in polarization will have the information about the geometric phase we are looking for.

Bitter and Dubber used a brilliant experimental setup in order to unveil the Berry phase contribution to polarization. They took a beam of neutrons travelling at a speed of 500 m/s, which was polarized up to the 97%.

This high degree of polarization meant that almost all the magnetic moments associated to the neutrons were all parallel to a given direction. The beam was, then, sent through a tube where an helical magnetic field was produced by a coil wrapped onto it (Figure 1.6).

The hamiltonian for the neutrons in this experiment is thus:

$$ H = \frac{p^2}{2m} - \mu \cdot \mathbf{B}. \quad (1.86) $$
where $p$ is the neutron momentum, $m$ its mass, while $\mu$ its magnetic dipole moment. We can neglect gravitational or electromagnetic interactions, so that the particle trajectories do not bend, and neutrons follow their original path.

In the center of mass frame of the neutron the magnetic dipole moment interacts with a magnetic field that traces one complete revolution around the origin. In this case the angle described by the tip of the vector representing the magnetic field is exactly $2\pi$.

In order to modify the value of this angle, an extra magnetic field coaxial to the tube could be added. Bitter and Dubbers then posed the following question: “Given that the particles are injected into the tube with a certain polarization, what would be the intensity of the beam as it leaves the experimental setup and gets probed by an output analyzer?” The interesting part is that this problem can be studied exactly and the Berry phase can be computed as a limiting case. In this experimental setup the adiabatic limit corresponds to the direction of the magnetic field changing slowly compared to its amplitude, or, more precisely to the precession frequency of the spin around the field. One can prove that the total phase after a travel in the tube, in the adiabatic limit, is:

$$\phi_t = bT - 2\pi,$$

where $b$ is the field strength times the gyromagnetic ratio of the neutrons, $T$ is the period associated to a single turn-around. We can interpret the above formula in these terms: the first contribution represents the dynamical phase, while the second one, which is time-independent, heavily relies on the path followed by the
Figure 1.7: The experimental results show a good agreement between the hypothesis of the Berry phase and the data obtained.

magnetic field. It is this latter that is interpreted as Berry’s phase, whose origin is purely geometrical. In fact, if we switch on the extra magnetic field, the coaxial one, we can modify the solid angle $2\pi(1 - \cos \theta)$ which is enclosed by the path, and consequently obtain different contributions as shown in (Figure 1.7).

So far we have discussed only one experimental evidence of geometric phases, probably the simplest one, which dealt with Berry’s phase. Moreover in this case the environment has to be considered classical (the magnetic field) and can be manipulated by the experimenter. In more realistic cases, the environment itself could be a quantum system and geometric phases can appear in molecular systems as a result of the interaction between electronic and rotational motions or of the interaction between electronic and vibrational motions. In these cases, in fact, a fictitious magnetic flux appear in the Born-Oppenheimer approximation, which, introducing gauge potential terms, gives rise to some geometric phases.

Moreover geometric phases can be associated with Bloch waves in crystalline solids and with adiabatic particle transport linked to polarization calculations for crystal dielectrics. So far, the most fascinating application of the geometric phase could
be considered the well-known quantum-Hall effect \cite{31, 32}. It is a quantum phenomenon involving two-dimensional electron systems in strong magnetic fields and low-temperatures. In the case of the integer quantum-Hall effect, the quantization of the Hall conductance can be explained in terms of a topological invariant: the Chern number.

Furthermore the concept of geometric phase has proved to be a fundamental tool in the study of spin-wave dynamics in itinerant magnets \cite{33}. Spin waves are collective modes of motion in the local magnetic moments in magnetized materials. The simplest approach to the problem is provided by the Heisenberg model, where the spins are bound to atomic sites. There are other cases where the itinerant picture is far more interesting: the spins are carried by Bloch states moving throughout the system. It is a matter of fact that the calculation of spin waves for itinerant-electron systems has been an undiscovered area in condensed matter physics. Geometric phases have proved to be essential in order to properly understand the underlying structures.

A lot of improvements have been made so far, and geometric phases have been studied in different contexts showing unexpected and surprising results. The variety of applications shows us how fertile is the field of geometric phases and who knows what we could expect in the next near future. For a complete review on geometric phases and a detailed description of the above cited results an excellent reference is \cite{34}.
Chapter 2

Self-Adjointness and Boundary Conditions

If one has really technically penetrated a subject, things that previously seemed in complete contrast, might be purely mathematical transformations of each other.

John von Neumann

2.1 An Introduction to Boundary problems: A free particle on an interval

In this section we would like to introduce the problem of self-adjoint extensions of Hermitian operators with a simple example provided by the momentum on an interval. Let \( p \) be the derivation operator on \( L^2(0,1) \):

\[
p\phi = -i \frac{d}{dx} \phi,
\]

\( D(p) = \{ \phi : \phi \in \mathcal{H}^1[0,1], \phi(0) = 0 = \phi(1) \} \).

The operator \( p \) describes the momentum of a particle in a one-dimensional box of unit length (\( \hbar = 1 \)). The box has impenetrable hard walls, so that the wave function is forced to vanish at the edges of the interval. \( \mathcal{H}^1[0,1] \) is the Sobolev space of square integrable functions whose distributional derivatives are square
integrable functions as well. For some more details about Sobolev spaces see Appendix A.

One can prove that the adjoint operator has the same functional form as in (2.1) but it is defined over a larger space, the whole $\mathcal{H}^1[0,1]$. $p$ is not essentially self-adjoint since:

$$e^{\pm x} \in D(p^*) \quad \text{and} \quad p^*(e^{\pm x}) = \mp ie^{\pm x},$$

(2.2)

but they do not belong to $D(p)$. Moreover one can prove that $p$ is closed. Summing up: $p$ is symmetric, closed but it is not self-adjoint. Now we would like to prove that $p$ admits self-adjoint extensions, and as we will see there are uncountably many, all of the form:

$$D(p_\alpha) = \{ \phi : \phi \in \mathcal{H}^1[0,1], \phi(1) = \alpha \phi(0) \}, \quad \alpha \in \mathbb{C}, \quad |\alpha| = 1,$$

(2.3)

$$p_\alpha = -i \frac{d}{dx}.$$

It is useful to note that all these extensions are restrictions of $p^*$, and that a $U(1)$ structure is hidden somewhere in the background. Figure 2.1 shows this: all self-adjoint extensions of $p$ are identified with elements of the circle, and all of them are restrictions of $p^*$.

In this and in the following paragraphs we will get a further insight on this. We now prove (2.3). Suppose $S$ is a symmetric extension of $p$, and since $D(S^*) \subset D(p^*)$ functions in $D(S^*)$ are absolutely continuous and the adjoint of $S$ acts on its...
domain as the adjoint of $p$. In the study of a characterization of $D(S^*)$ one starts by fixing $\phi \in D(S)$ and $\psi \in D(S^*)$ and tries to get some information from:

$$0 = \langle S\phi, \psi \rangle - \langle \phi, S^*\psi \rangle = \phi(1)\psi(1) - \phi(0)\psi(0),$$  \hspace{1cm} (2.4)$$

where in the last equality we used the integration by parts formula, which still holds for absolutely continuous functions. In the case $S = p$ the boundary conditions (Dirichlet) in $D(p)$ are so restrictive that one needs no boundary conditions in $D(p^*)$ in order to satisfy (2.4) and this is mainly the reason why $p$ is not self-adjoint.

Thus we have proved that the momentum of a particle in a box cannot be represented by a self-adjoint operator and, according to the axioms of quantum mechanics, it is not an observable. Pathologies of quantum Hamiltonians are reflected in their classical counterparts and in the solution of the associated classical dynamics \[35\]. The classical counterpart of our problem is provided by a free particle bouncing elastically between two rigid walls. In this particular case any physical trajectory has a definite value of energy ($p^2/2m$), while the momentum changes periodically between $+p$ and $-p$ (see Figure 2.2). As proved in \[36\] this is reflected in the lack of self-adjointness of the operator $p$. In fact in quantum mechanics if we
suppose that the particle has finite momentum $+k$, then, its associated eigenfunction will be $e^{ikx}$ which does not vanish at the border, that is, it does not belong to $D(p)$; the same holds for $-k$. Another interesting perspective can be provided by a semiclassical approach: if we consider the approach to quantization by Bohr and Sommerfeld we know that the eigenfunction associated to a certain system must be settled on a fixed momentum orbit in the phase space. But as one can see in Figure 2.2, the orbit is uniquely fixed by the energy $p^2/2m$ but two values of $p$ can alternatively be chosen.

We have thus understood that we need less stringent boundary conditions than Dirichlet’s ones so that solving (2.4) gives the same boundary conditions on $D(S^*)$. With this end in view let $S$ be a self-adjoint extension of $p$ and suppose $\phi \in D(S) \setminus D(p)$, then (2.4) requires that $|\phi(1)|^2 = |\phi(0)|^2$, and since $\phi \notin D(p)$, $\phi(0) \neq 0$, so there exists an $\alpha \in \mathbb{C}$ and $|\alpha| = 1$ such that $\phi(1) - \alpha \phi(0) = 0$. If we take any other $\psi \in D(S)$, we find that $\psi(1) - \alpha \psi(0) = 0$ with the same identical $\alpha$. Thus, $S \subset p_\alpha$, where $p_\alpha$ is defined in (2.3). Moreover $S = p_\alpha$ for some $\alpha$ since $S$ is self-adjoint and $p_\alpha$ is symmetric.

Next we prove that $p_\alpha$ is self-adjoint for each $\alpha$. In order to show this we choose $\phi \in D(p_\alpha)$ and $\psi \in D(p_\alpha^*)$. Then (2.4) leads to the following condition:

$$\overline{\alpha \phi(0)} \psi(1) - \overline{\phi(0)} \psi(0) = 0,$$

which gives $\psi \in D(p_\alpha)$.

Therefore we have proved that $D(p_\alpha) = D(p_\alpha^*)$, that is $p_\alpha$ is self-adjoint for every $\alpha$, so that all self-adjoint extensions of $p$ belong to the set $\{p_\alpha | \alpha \in \mathbb{C}, |\alpha| = 1\}$.

In the next section we will show how to get the same result with the study of deficiency subspaces. Before starting our summary of von Neumann’s theory of self-adjoint extensions, we would like to stress that every self-adjoint extension corresponds to a different physical situation, so that all the domain machinery which might seem artificial and a technical inconvenience at the very beginning, becomes much more natural for the description of quantum physical systems.
2.2 Physical Interpretation of Boundary Conditions: A First Look

Boundary conditions are not some artificial tool we need to plug in our treatment of self-adjoint extensions, but rather a mathematical representation of some physical situations.

It is well known, in fact, that a quantum particle confined in an impenetrable box can be described in terms of a Laplacian defined over some suitable domain where Dirichlet boundary conditions are imposed; that is to say functions vanishing at the box’s walls. In fact in this specific case the particle is confined into the box and cannot escape, so that the only way of treating this problem is to impose the vanishing of the wavefunction at the border.

But as we have already pointed out, the momentum operator with Dirichlet boundary conditions does not provide a self-adjoint operator, although the Hamiltonian, i.e. $p^2$, is an observable. We now try to solve this mystery by showing why this happens and how one can physically interpret boundary conditions.

We consider a wave packet $\phi(x)$ defined in $[0,1]$ and compactly supported. This actually means that $\phi(x)$ is zero near the border of $[0,1]$. Next we perform a translation of a small enough quantity $y$ of the wave packet to the right as shown in Figure 2.3. Of course we choose $y$ so that the translated wave packet does...
not reach the boundary as well. In section [3.2.1] we will explicitly show that translations can be represented by a family of operators:

\[ U(y) : \phi(x) \rightarrow \phi(x - y), \]  

(2.6)

whose generator, is given by the momentum operator according to Stone’s theorem. So we can physically think of the momentum as the generator of translations in the compact interval such that the translated function is still compactly supported in the same interval. From the general theory of self-adjoint operators we have learnt that \(-id/dx\) is a symmetric operator on \(C^1_0(0,1)\) whose closure is given by (2.1).

But as we have already stated \(p\) is not self-adjoint and the reason should be now clearer in light of our discussion about translations in the interval. By implementing only translations of functions which are zero near the endpoints we are discarding an important physical feature of our system: the boundaries. In other words we are not taking into account what happens when the wave-packet reaches the box.

Since we need translations to be represented by a unitary group, then the preservation of probability requires that:

\[ \int_0^1 |\phi(x - y)|^2 dx = \int_0^1 |\phi(x)|^2 dx. \]  

(2.7)

Roughly speaking we are requiring that what comes out at one end of the border must come back in at the other. As we are going to mention later this basically means that we are deforming the interval \([0,1]\) into a circle.

We still have the freedom of choosing the phase of the wave packet as it comes back in at the other end. The different implementations of translations are thus specified by unitary complex numbers \(\alpha\) and by requiring that wave packets do satisfy the boundary conditions in (2.3). The translation of the wave packet is thus given by \(e^{-iyp_\alpha}\), so that we do understand that different self-adjoint extensions correspond to different physical situations.
2.3 Von Neumann’s Theorem

In this section we follow \([37–39]\) in order to investigate the nature of self-adjoint extensions of symmetric operators. In quantum mechanics we need self-adjoint operators for several physical reasons: we need to preserve probability and by Wigner’s theorem all symmetries which preserve probability amplitudes must be implemented either by unitary or by antiunitary operators on a Hilbert space. Moreover all unitary groups are given, according to Stone’s theorem, as “exponentials” of self-adjoint operators, which represent the generators of the action provided by the corrispective unitary operators on the Hilbert space. So one reason for self-adjointness relies on the dynamics of a system. Another reason is kinematic: the values of an observable measured in experiments are real numbers.

In the mathematical foundations of quantum mechanics we are brought to think about observables in terms of linear operators on Hilbert spaces, and their values are linked to their spectral properties. It can be shown that, in general, Hermitian operators do not have a spectrum which is purely real, so that no physical interpretation can be given. Instead, the spectrum of a self-adjoint operator is purely real, so that it is rather reasonable to demand that observables may be represented in terms of self-adjoint operators.

Let us recall some well-known results about self-adjoint extensions of operators:

Let \( T \) be a densely defined symmetric operator (more concisely Hermitian) we can define the Cayley transform of \( T \):

\[
U(T) : \text{Ran}(T + i \mathbb{I}) \to \text{Ran}(T - i \mathbb{I}), \quad U(T) = (T - i \mathbb{I})(T + i \mathbb{I})^{-1}.
\] (2.8)

It is easy to prove that this map is both isometric and linear. We now define the deficiency subspaces as:

\[
K_\pm(T) = \text{Ker}(T^* \pm i \mathbb{I}) = \text{Ran}(T \mp i \mathbb{I}),
\] (2.9)

and their respective dimensions, \( n_\pm = \dim K_\pm(T) \), are known as deficiency indices, since, as we will see soon, they quantify the lack of self-adjointness of an operator. Coherently with what defined above one can prove that a symmetric operator is self-adjoint if and only if the \( \text{Ran}(T + i \mathbb{I}) = \text{Ran}(T - i \mathbb{I}) = \mathcal{H} \), that is its Cayley transform is a unitary operator. Moreover it can be proved that if we consider a linear isometry that extends the Cayley transform of \( T \), then, there
exist a Hermitian operator that extends $T$ and whose Cayley transform extends the given linear isometry. Then, combining these two results we can translate the search for self-adjoint extensions of Hermitian operators into the search for unitary extensions of Cayley transforms.

A little remark: all self-adjoint extensions of an operator (which are obviously closed) will lie between its smallest and biggest closed extensions that is its closure and its adjoint. Let us now try to understand the main result of von Neumann about the existence of self-adjoint extensions of Hermitian operators. Let $T$ be a closed and an Hermiotian operator, then we can decompose our Hilbert space into two mutually orthogonal subspaces:

$$\mathcal{H} = \text{Ran}(T \pm i \mathbb{I}) \oplus \text{Ran}(T \pm i \mathbb{I})^\perp = \text{Ran}(T \pm i \mathbb{I}) \oplus K_+(T), \quad (2.10)$$

and we know that $U(T)$ is an isometry between $\text{Ran}(T + i \mathbb{I})$ and $\text{Ran}(T - i \mathbb{I})$. In order to find a self-adjoint extension of $T$ one needs to extend $T$ to a certain $\tilde{T}$ so that $\text{Ran}(\tilde{T} \pm i \mathbb{I}) = \mathcal{H}$, that is $U(\tilde{T})$ is unitary on $\mathcal{H}$. Of course, this requires $n_+ = n_-$, which is the core of von Neumann’s theorem:

**Theorem 2.1.** Let $T$ be a Hermitian operator and $\tilde{T}$ its closure. Then:

1. $D(T^*) = D(\tilde{T}) \oplus_{T^*} K_+(T) \oplus_{T^*} K_-(T)$;
2. $T$ is essentially self-adjoint $\Leftrightarrow n_+ = n_- = 0$;
3. $T$ admits self-adjoint extensions $\Leftrightarrow n_+ = n_-$. There exist a 1-1 correspondence between self-adjoint extensions of $T$ and unitary operators between $K_-(T)$ and $K_+(T)$ (infinite of them if $n_+ = n_- \geq 1$; one and only one if $n_+ = n_- = 0$).

The above direct sum $\oplus_{T^*}$ has to be considered in the topology provided by the following scalar product:

$$\langle \phi, \psi \rangle_{T^*} = \langle \phi, \psi \rangle + \langle T^*\phi, T^*\psi \rangle \quad \forall \phi, \psi \in D(T^*). \quad (2.11)$$

We will not provide a proof of the Theorem which can be easily found in [37,39], but we would like to explicitly show the non-constructive spirit of the theorem, which does not show how to build from scratch self-adjoint extensions of operators.
Since \( n_+ = n_- \) then the two deficiency subspaces are unitarily equivalent, that is:

\[
\exists \mathcal{U} : K_- \rightarrow K_+,
\]

(2.12)
such that \( \mathcal{U} \) is a unitary operator between the two Hilbert subspaces. This unitary operator is not unique, and as we will shortly see, here lies the non-uniqueness of self-adjoint extensions and the non-constructive behavior of the theorem.

In order to make use of the 1-1 correspondence between self-adjoint operators and unitary Cayley transforms we need to extend \( \mathcal{U}(T) \), which is solely an isometry as long as \( T \) is Hermitian. Thus, we consider \( \mathcal{U}(\overline{T}) \), the Cayley transform of the closure of \( T \):

\[
\mathcal{U}(\overline{T}) : \text{Ran}(T + iI) \rightarrow \text{Ran}(T - iI),
\]

(2.13)
and we compose it with \( \mathcal{U} \), in order to have:

\[
\tilde{\mathcal{U}} := \mathcal{U}(T) \oplus \mathcal{U} : \text{Ran}(T + iI) \oplus K_-(T) \rightarrow \text{Ran}(T - iI) \oplus K_+(T).
\]

(2.14)
\( \tilde{\mathcal{U}} \) is of course an isometry, it extends \( \mathcal{U}(T) \) and most importantly it is a unitary operator since \( \text{Ran}(T + iI) \oplus K_-(T) = \mathcal{H} = \text{Ran}(T - iI) \oplus K_+(T) \). From the discussion above, then, there exist a self-adjoint extension of \( T \) whose Cayley transform is \( \tilde{\mathcal{U}} \). We would like to stress that from (2.14) it is again evident that, when \( n_+ = n_- \geq 1 \), \( T \) will admit infinitely many self-adjoint extensions, since \( \mathcal{U}(T) \) is uniquely determined but \( \mathcal{U} \) is not.

### 2.4 Boundary Forms and Self-Adjoint Extensions

Von Neumann’s theory gives a general formulation of the problem of self-adjoint extensions but, as discussed above, does not provide a way to explicitly build them up. Before diving into the theory of boundary triples, which generalizes the notion of boundary values in functional spaces, we would like to show how self-adjoint extensions can be constructed as restrictions of \( T^* \) over domains where a certain sesquilinear form identically vanishes. Given \( T \) Hermitian, we define the following sesquilinear form:

\[
\Gamma_{T^*} : D(T^*) \times D(T^*) \rightarrow \mathbb{C},
\]

\[
\Gamma_{T^*}(\xi, \eta) := \langle T^*\xi, \eta \rangle - \langle \xi, T^*\eta \rangle, \quad \forall \xi, \eta \in D(T^*).
\]

(2.15)
One can use the boundary form to characterize the closure of $T$, that is:

$$\xi \in D(T) \iff \Gamma_T(\xi, \phi) = 0, \quad \forall \phi \in D(T^*). \quad (2.16)$$

Moreover the boundary form can be used as a measure of “lack of self-adjointness” of the adjoint operator $T^*$, since one can prove that $T^*$ is self-adjoint (or equivalently $T$ essentially self-adjoint) if and only if:

$$\Gamma_{T^*}(\xi, \eta) = 0, \quad \forall \xi, \eta \in D(T^*). \quad (2.17)$$

Thus as a general rule in the search of self-adjoint extensions of Hermitian operator one starts investigating the closure of $T$ and checks whether condition (2.17) is satisfied or not. In the affirmative case, we have found that our operator is essentially self-adjoint, which means that $T$ admits one and only one self-adjoint extension given by its closure, which is its smallest closed extension. In the negative case, one needs to study with further insight the nature of boundary forms. In fact, their strength lies in the possibility of characterizing self-adjoint extensions as restrictions of $T^*$ on suitable domains where the form vanishes. One may get a feeling for this by noting that, given a Hermitian operator, the domain of its closure can be written as:

$$D(T) = \{ \xi \in D(T^*) : \Gamma_{T^*}(\xi, \eta) = 0, \quad \forall \eta \in K(T) \}. \quad (2.18)$$

Moreover it is easy to understand that the non vanishing of $\Gamma$ is related to the deficiency subspaces; in fact if we fix $\zeta_1$ and $\zeta_2$ in $D(T^*)$ one can use von Neumann’s decomposition so that:

$$\zeta_1 = \eta_1 + \eta_1^+ + \eta_1^-,$$
$$\zeta_2 = \eta_2 + \eta_2^+ + \eta_2^-,$$  

with $\eta_1, \eta_2 \in D(T), \eta_1^+, \eta_2^+ \in K_+(T)$ and $\eta_1^-, \eta_2^- \in K_-(T)$. Using this decomposition and the characterization of $T$ in terms of the boundary form one finds that:

$$\Gamma_{T^*}(\zeta_1, \zeta_2) = 2i \left( \langle \eta_1^+, \eta_2^+ \rangle - \langle \eta_1^-, \eta_2^- \rangle \right). \quad (2.21)$$

So as expected, the essential ingredient in the study of self-adjoint extensions of Hermitian operators is given by the deficiency subspaces, where in general the
boundary form does not necessarily vanish. Let us suppose that $T$ admits self-adjoint extensions, that is $n_+ = n_-$. From von Neumann’s theory we know that each self-adjoint extension is in a one-to-one correspondence with a unitary operator acting between the deficiency subspaces. If we set $T_{U}$ the corresponding self-adjoint operator then one can prove \cite{39} that (actually this result suitably re-written holds in a more general case of Hermitian extensions whose Cayley transform is built as in (2.14)):

$$D(T_{U}) = \{ \eta = \zeta + \eta_- - U\eta_- : \zeta \in D(T), \eta_- \in K_-(T) \}, \quad (2.22)$$

$$T_{U} = T^*|_{D(T_{U})}.$$ 

Then it follows that the boundary form identically vanishes on $D(T_{U})$, and, moreover, each self-adjoint extension of $T$ is given by

$$D(T_{U}) = \{ \xi \in D(T^*) : \Gamma_{T^*}(\xi, \eta_- - U\eta_-) = 0, \forall \eta_- \in K_-(T) \}. \quad (2.23)$$

So far we have outlined the general setting. In Appendix C we show that the boundary form associated to the Laplacian can be recast in terms of the Wronskian.

### 2.5 Boundary Triples

We now introduce a more general tool which can be useful while dealing with the search of self-adjoint extensions. We will show how this naturally arises from von Neumann’s theory and extends the latter. Von Neumann’s theory and the use of boundary forms are helpful when studying differential operators, but what could one state about self-adjoint extensions of Hermitian operators, which are not in general differential operators? A plausible answer could be given by boundary triples, which are a natural generalization of the notion of boundary values in functional spaces. This idea is not new, anticipations, in fact, can be found in \cite{40} and \cite{41}. For a modern review on the topic see for instance \cite{42}.

Let $T$ be a Hermitian operator with equal deficiency indices. Let $h$ be a Hilbert space and take:

$$\rho_1, \rho_2 : D(T^*) \xrightarrow{\text{lim}} h, \quad (2.24)$$
whose ranges are dense in $h$:

$$\text{Ran}(\rho_1) = h = \text{Ran}(\rho_2),$$

so that they satisfy the following condition:

$$a\Gamma_{T^*} = \langle \rho_1(\xi), \rho_1(\eta) \rangle - \langle \rho_2(\xi), \rho_2(\eta) \rangle, \quad \forall \xi, \eta \in D(T^*),$$

where $a \in \mathbb{C}$, $a \neq 0$, and $\Gamma_{T^*}$ is the boundary form defined in section 2.4. A triple $(h, \rho_1, \rho_2)$ that satisfies the above conditions is called a boundary triple.

Since $T$ has equal deficiency indices, then by von Neumann’s theorem it admits self-adjoint extensions. The main objective of this paragraph is to show that these extensions can be built up once suitable boundary triples have been given.

Recall that from (2.21) the non-vanishing of the boundary form is due to non-trivial deficiency subspaces, so that one may choose either $h = K_+(T)$ or $h = K_-(T)$, and once more by von Neumann’s theorem all self-adjoint extensions are in a one-to-one correspondence with unitary operators $U : K_-(T) \rightarrow K_+(T)$. Moreover, it could be useful to consider $h$ with the same dimension of either one of the two deficiency subspaces. The latter statement is enforced by the fact that two Hilbert spaces are unitarily equivalent if and only if they have the same dimension.

We now need to mix some ingredients in order to find a condition that links self-adjoint extensions with unitary operators acting between $K_+(T)$ and $K_-(T)$. First of all we have already seen that self-adjoint extensions of $T$ are restrictions of its adjoint to suitable domains where the boundary form identically vanishes. Secondly, given a boundary triple for $T$, (2.26) holds so that these domains are related to isometric maps in $h$ such that $\rho_2(\xi) = U\rho_1(\xi)$. One can prove that such isometries are linear operators which can eventually be extended to unitary operators.

These remarks naturally lead to the following theorem:

**Theorem 2.2.** Let $T$ be a Hermitian operator with equal deficiency indices. If $(h, \rho_1, \rho_2)$ is a boundary triple for $T$, then the self-adjoint extensions $T_U$ of $T$ are:

$$D(T_U) = \{ \xi \in D(T^*) : \rho_2(\xi) = U\rho_1(\xi) \}, \quad T_U\xi = T^*\xi,$$

for every unitary operator $U : h \rightarrow h$. 


We now provide an example which will shed some light on the usefulness of this construction.

### 2.5.1 A free particle on the interval (one more time)

Let us return to our free particle on the interval and as we have already seen the Laplacian operator cannot be self-adjoint unless some suitable boundary conditions are imposed. In fact, if we take:

\[ H\psi = -\psi'', \quad D(H) = C_0^\infty(0,1), \quad (2.28) \]

its adjoint will be defined over the larger space \( \mathcal{H}^2[0,1] \), and will have the same functional form of (2.28) on its domain. Next, we study its deficiency indices, by solving the differential equations:

\[ (H^* \pm iI)\psi = 0, \quad (2.29) \]

and from the theory of ordinary differential equations, one finds that the set of linearly independent solutions is bidimensional so that: \( n_+ = n_- = 2 \), thus \( K_+(T) \simeq K_+(T) \simeq \mathbb{C}^2 \) are isomorphic Hilbert spaces. Consequently the Laplacian operator admits self-adjoint extensions, that we are going to build up once a boundary triple has been defined.

We choose \( h = \mathbb{C}^2 \) and define:

\[ \rho_1 : D(H^*) \to \mathbb{C}^2 : \psi \mapsto \begin{pmatrix} \psi(0) - i\psi'(0) \\ \psi(1) + i\psi'(1) \end{pmatrix}, \quad (2.30) \]

\[ \rho_2 : D(H^*) \to \mathbb{C}^2 : \psi \mapsto \begin{pmatrix} \psi(0) + i\psi'(0) \\ \psi(1) - i\psi'(1) \end{pmatrix}, \quad (2.31) \]

where these functions are well defined since \( C^2[0,1] \subset \mathcal{H}^2[0,1] \). It is easy to prove that \( \text{Ran}\rho_1 = \text{Ran}\rho_1 = \mathbb{C}^2 = \text{Ran}\rho_2 = \text{Ran}\rho_2 \), and moreover equation (2.26) holds:

\[ \langle \rho_1(\xi), \rho_1(\eta) \rangle - \langle \rho_2(\xi), \rho_2(\eta) \rangle = 2i \Gamma_{H^*}(\xi, \eta). \quad (2.32) \]
So \((\mathbb{C}^2, \rho_1, \rho_2)\) is a boundary triple for \(H\), and by Theorem 2.2 the domains of self-adjointness are characterized by unitary \(2 \times 2\) matrices:

\[
\mathcal{U} = e^{-i\theta} \begin{pmatrix} \bar{a} & \bar{b} \\ -b & a \end{pmatrix}, \quad \theta \in [0, 2\pi), \quad a, b \in \mathbb{C}, \quad |a|^2 + |b|^2 = 1,
\]

so that \(\rho_2(\xi) = \mathcal{U} \rho_1(\xi), \forall \xi \in D(H^*)\), that is:

\[
(\mathbb{I} - \mathcal{U}) \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} = i (\mathbb{I} + \mathcal{U}) \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix}.
\]

In the end, all self-adjoint extensions of (2.28) are given by:

\[
D(H_\mathcal{U}) = \left\{ \psi \in H^2[0, 1] : (\mathbb{I} - \mathcal{U}) \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} = i (\mathbb{I} + \mathcal{U}) \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix} \right\}, \quad H_\mathcal{U} \psi = -\psi''.
\]

By choosing particular unitary matrices one can pick out some well-known boundary conditions:

\[
\begin{align*}
\mathcal{U} &= -\mathbb{I}, \quad \psi(0) = 0 = \psi(1), \quad \text{Dirichlet}; \\
\mathcal{U} &= \mathbb{I}, \quad \psi'(0) = 0 = \psi'(1), \quad \text{Neumann}; \\
\mathcal{U} &= \sigma_1, \quad \psi(0) = \psi(1), \quad \psi'(0) = \psi'(1), \quad \text{periodic}; \\
\mathcal{U} &= -\sigma_1, \quad \psi(0) = -\psi(1), \quad \psi'(0) = -\psi'(1), \quad \text{antiperiodic}.
\end{align*}
\]

The same results can be obtained by considering only the vanishing of the boundary form as illustrated in the previous paragraph.

In the following we will be interested in a particular subclass of boundary conditions, which we are going to discuss. If we consider the following matrix \(\mathcal{U}\), with \(\eta \in \mathbb{C}_\infty = \mathbb{C} \cup \{\infty\}\):

\[
\mathcal{U} = \begin{pmatrix} |\eta|^2 - 1 & 2\eta \\ 1 + |\eta|^2 & 1 - |\eta|^2 \end{pmatrix}, \quad \eta \in \mathbb{C} \cup \{\infty\}, \quad |\eta|^2 + 1 = 1,
\]

it is easy to prove that it is a unitary matrix, and that it generates the following boundary conditions:

\[
\begin{align*}
\psi(0) &= \eta \psi(1), \\
\bar{\eta} \psi'(0) &= \psi'(1).
\end{align*}
\]
For \( \eta = \pm 1 \) we obtain periodic and antiperiodic boundary conditions, while for \( \eta = 0 \) or \( \eta = \infty \) mixed Dirichlet and Neumann. All boundary conditions which do not mix functions with derivatives are given by the subset of \( U(2) \) made up by \( \{ U(\eta) \}_{\eta \in \mathbb{C}_\infty} \) and pure Dirichlet or Neumann boundary conditions. In fact, take non-mixed boundary conditions in form of the following linear system:

\[
\begin{align*}
\alpha \psi(0) + \beta \psi(1) &= 0, \\
\gamma \psi'(0) + \delta \psi'(1) &= 0,
\end{align*}
\]  

where \( \alpha, \beta, \gamma, \delta \in \mathbb{C} \). We would like to determine which conditions have to be satisfied by the former four parameters for the linear system to represent a suitable self-adjoint extension of the Laplacian on the interval \([0, 1]\). From the theory described in section 2.4, we have learnt that the system in (2.43) can represent a self-adjoint extension of the operator if and only if the boundary form identically vanishes on the subspace of the boundary conditions. For a discussion on the explicit expression of \( \Gamma_{H^*} \) and its link to the Wronskian of a second order differential equation see Appendix C. Thus, imposing that \( \Gamma_{H^*} \):

\[
\Gamma_{H^*}(\phi, \psi) = \overline{\phi(1)\psi'}(1) - \overline{\phi'(1)\psi}(1) - \overline{\phi(0)\psi'}(0) + \overline{\phi'(0)\psi}(0), \tag{2.44}
\]

vanishes identically on the subspace spanned by (2.43) we have that:

\[
\begin{align*}
\psi(0) &= -\frac{\beta}{\alpha} \psi(1), \\
\psi'(0) &= -\frac{\delta}{\gamma} \psi'(1), \\
\frac{\beta}{\alpha} \frac{\delta}{\gamma} &= 1,
\end{align*}
\]  

which is nothing but (2.42), if we define:

\[
-\frac{\beta}{\alpha} = \eta. \tag{2.46}
\]

In addition to that we could have other two admissible cases:

\[
\begin{align*}
\psi(0) &= 0, \\
\psi'(1) &= 0,
\end{align*}
\]  

or:

\[
\begin{align*}
\psi(1) &= 0, \\
\psi'(0) &= 0.
\end{align*}
\]
These latter correspond to a Dirichlet condition on one end-point, and to a Neumann condition on the other. The first one can be recovered from (2.43), if $\eta = 0$, while the second one if $\eta = \infty$.

We stress that pure Dirichlet or Neumann boundary conditions on both end-points are not parametrized in (2.43). So that the set of boundary conditions which do not mix functions with derivatives is given by the set:

$$\{U(\eta)_{\eta \in C_\infty}, I, -I\}. \quad (2.49)$$

Finally, it is worth noticing that the set $\{U(\eta)\}_{\eta \in C_\infty}$ does not form a subgroup of $U(2)$, since for all $\eta_1, \eta_2 \in C$:

$$U(\eta_1)U(\eta_2) \neq U(\eta_1\eta_2). \quad (2.50)$$

### 2.6 Physical Interpretation of Boundary Conditions: A scattering approach

In the previous section we found all self-adjoint extensions of the Laplacian on an interval, and in particular we met again with Dirichlet and Neumann conditions. It is legitimate to ask what would be the physical meaning of these conditions. In section 2.2 we analyzed the role of boundary conditions in the light of unitary preservation, and stressed the necessity of deforming the interval topology into the circle one, in order to make the transition “what comes out from one end must return to the other” a physical one (Figure 2.4, Figure 2.5).

We would like to show, through the use of scattering techniques, what is the physical meaning of the requests made so far, e.g. the vanishing of the wave function or of its derivative at one endpoint. We take the Laplacian defined over its maximal domain on an interval $[0, 1]$, that is $H^2[0, 1]$, and study what happens in a neighbourhood of $0$. In order to do that we consider a plane wave $e^{-ikx}$, which is in $H^2[0, 1]$, coming from the right (region I), which in part gets reflected (region I) and in part transmitted (region II). (Figure 2.6)
Figure 2.4: Physical bending of an interval.

Figure 2.5: After the bending, the functions defined over the interval transform as in figure.
Let $R$ be the reflection coefficient and $T$ the transmission one, so that the wavefunction can be written as:

$$\psi(x) = \begin{cases} 
\psi_I(x) = e^{-ikx} + Re^{ikx} & x \in I, \\
\psi_{II}(x) = Te^{-ikx} & x \in II 
\end{cases} \quad (2.51)$$

We start analyzing the physical meaning of $\psi(0) = 0$. By imposing this condition in (2.51) we find that:

$$\begin{cases} 
R = -1 \\
T = 0
\end{cases} \quad (2.52)$$

Physically this means that the plane wave scatters against a hard wall, no transmission takes place, and it is completely reflected. In the reflection process it acquires a $\pi$ phase like in the classical case of scattering of light against a mirror. In the physical interpretation of $\psi(0) = 0$, we can always think of bending our interval into a ring with a junction that consists of an infinitely high wall.

Next we move on to $\psi'(0) = 0$ and find that:

$$\begin{cases} 
R = 1 \\
T = 0
\end{cases} \quad (2.53)$$

In this case as well, the incoming wave gets completely reflected by a hard wall, but in this case in the reflection process it does not acquire any additional phase.

In the next chapter we will prove that there exists a non trivial geometric phase for a free particle described by a Laplacian with the following boundary conditions:

$$\psi(0) = \eta \psi(1), \quad \eta \psi'(0) = \psi'(1). \quad (2.54)$$

We have already remarked that in order to give a physical meaning to our boundary problems we need to bend our segment so that the interval ends are brought close to each other to form the two sides of a junction, so that the conditions we need to impose are:

$$\begin{cases} 
\psi_I(0) = \eta \psi_{II}(0) \\
\eta \psi'_I(0) = \psi'_{II}(0)
\end{cases} \quad (2.55)$$
Section 2.5: Scattering of a plane wave $e^{-ikx}$ against one of the boundary’s ends.

which lead to the following coefficients:

$$R = \frac{|\eta|^2 - 1}{1 + |\eta|^2},$$  \hspace{1cm} (2.56)

$$T = \frac{2\pi}{1 + |\eta|^2}.$$  \hspace{1cm} (2.57)

In the periodic case, $\eta = 1$, where we can identify the interval ends, the incident wave is completely transmitted through the junction, that is the particle is freely moving on a circle. In the antiperiodic case, instead, that is $\eta = -1$, again the wave is completely transmitted, but by crossing the junction it acquires an additional $\pi$ phase.

It is highly remarkable that the coefficients found above are the same that we already found in the inspection of self-adjoint extensions of the Laplacian on the interval, that is:

$$\mathcal{U} = \begin{pmatrix} R & T^* \\ T & -R \end{pmatrix}.$$  \hspace{1cm} (2.58)

It is worth noticing that in the case studied above both $R$ and $T$ were independent of $k$. However, if we had started from conditions mixing functions and derivatives as:

$$\psi(0) = \eta \psi'(1),$$  \hspace{1cm} (2.59)
then the reflection and transmission coefficients would explicitly depend on the wave number.
Chapter 3

Moving Walls and Geometric Phases

3.1 Boundary Conditions

In chapter one we developed some geometrical techniques useful in the study of geometric phases in quantum systems. In chapter two, instead, we discussed how to build up self-adjoint extensions of Hermitian operators helped by boundary conditions on suitable domains. It is time to mix the ingredients and to reveal the existence of geometric phases in a quantum mechanical system: a free particle in a box with moving boundaries. See Figure 3.1.

The problem of the quantum bouncer dates back to 1949, when Enrico Fermi [43], proposed a model for the production of cosmic rays. Particles are originated and accelerated by collisions against varying magnetic fields. Afterwards in 1961, Ulam [44] reconsidered Fermi’s problem and introduced the Fermi accelerator where a particle bounces back and forth between two moving walls. Since then this problem has been studied from different perspectives, ranging from numerical solutions of the equations involved (for example [45]) to applications in the context of the dynamical version of the Casimir effect [46].
The problem was studied in [47] for the case of hard walls with Dirichlet boundary conditions. Here we will extend that analysis to more general boundary conditions, in order to get a nontrivial geometric phase.

Let us consider a free particle in the one dimensional box

\[ I_{l,a} = [a - l/2, a + l/2], \tag{3.1} \]

with \( a \in \mathbb{R}, \ l > 0 \). The Hilbert space is \( L^2(I_{l,a}) \), the space of square integrable functions on the interval \( I_{l,a} \). Its Hamiltonian is

\[ H = \frac{p^2}{2m}, \tag{3.2} \]

with domain

\[ D_{l,a} = \left\{ \psi \in \mathcal{H}^2(I_{l,a}) : \ \psi \left( a - \frac{l}{2} \right) = \eta \psi \left( a + \frac{l}{2} \right) , \ \bar{\eta} \psi' \left( a - \frac{l}{2} \right) = \psi' \left( a + \frac{l}{2} \right) \right\}, \tag{3.3} \]

where \( \eta \) is a fixed complex number, and \( \mathcal{H}^2(I_{l,a}) \) is the second Sobolev space of square integrable functions on \( I_{l,a} \), whose (first and) second derivatives are square integrable functions as well. The main results about Sobolev spaces are recalled in Appendix A.

In chapter 2, and in particular in section 2.5.1, we proved that the above boundary conditions yield a good self-adjoint extension of the Laplacian on an interval. In addition to that, these boundary conditions do not mix the values of the functions on the border with their derivatives. In the scattering interpretation of boundary conditions, as already discussed in section 2.6, this means that the reflection and
transmission coefficients do not depend on the wave number of the scattering plane waves. In the following we will see that these are the only boundary conditions which are invariant under dilations, a crucial property for what we are going to investigate.

Now we want to consider the problem of moving boundaries, so that the Hamiltonian will vary in time through the dependence of the parameters on time: \( t \mapsto a(t) \) and \( t \mapsto l(t) \) \((l(t) > l_0 > 0)\), which we will suppose smooth. Clearly this is not an easy problem to tackle, since we have a family of operators defined over different domains and we would like to find both its spectral decomposition (which of course will depend on \( a \) and \( l \)) and, eventually, the time evolution it determines. The latter, in order to have a meaning, needs further specification since the Hilbert space itself changes with time, and we need to compare vectors from different Hilbert spaces.

With this end in view we embed \( L^2(I_{l,a}) \) into \( L^2(\mathbb{R}) \) in the following way:

\[
L^2(\mathbb{R}) = L^2(I_{l,a}) \oplus L^2(\mathbb{R} \setminus I_{l,a}),
\]

so that we can consider the extension of the Hamiltonians defined above as:

\[
H(l,a) = \frac{p^2}{2m} + l(a,0),
\]

where the embedding and the direct sum obviously depend on \( l \) and \( a \). The action of \( H(l,a) \) is given by \( H(l,a)(\psi + \phi) = -\frac{1}{2m} \psi'' + 0 \phi, \forall \psi \in D_{l,a} \) and \( \forall \phi \in L^2(\mathbb{R} \setminus I_{l,a})\).

Our problem with varying domains can be unitarily mapped into a fixed domain one, so that it is easier to determine its spectral decomposition. Afterwards, we will be able to bijectively (and isometrically) return to our initial problem.

### 3.2 The Transformation

In this section, following [47] we show how to reduce our “moving walls” problem into a fixed domain one.

The composition of a translation \( x \to x - a \) and of a subsequent dilation \( x \to x/l \) maps the interval \( I_{l,a} \) into \( I = I_{1,0} = [-\frac{1}{2}, \frac{1}{2}] \), which does not depend on \( a \) and \( l \). The above transformations need to be lifted on \( L^2(\mathbb{R}) \), but this process is not
unique. We are going to prove that an admissible lifting of both actions can be implemented by:

\[(T(a)\psi)(x) = \psi(x - a), \quad (D(s)\psi)(x) = e^{-s/2}\psi(e^{-s}x),\]  

(3.6)

and that both \(a \in \mathbb{R} \to T(a)\) and \(s = \ln l \in \mathbb{R} \to D(s)\) form (separately) a one-parameter strongly continuous unitary group. In order to make the expression \(\ln l\) meaningful, from now on we are going to identify \(l\) with a pure number given by the ratio of the actual length of the box and a unitary length.

We recall that a strongly continuous one-parameter group is a family of unitary operators \(\{U(t) : t \in \mathbb{R}\}\) on a Hilbert space \(\mathcal{H}\) such that:

1. \(U(t)U(s) = U(t + s) \quad \forall t, s \in \mathbb{R},\)

2. \(\lim_{h \to 0} U(t + h)\psi = U(t)\psi \quad \forall \psi \in \mathcal{H}, \forall t \in \mathbb{R}.\)

The first requirement states that \(U\) is a group homomorphism of the underlying additive group \(\mathbb{R}\) into the group of unitary operators on \(\mathcal{H}\). As a consequence one can prove that:

- \(U(0) = I,\)
- \(U(-t) = U(t)^{-1} = U^*(t) \quad \forall t \in \mathbb{R}.\)
The second requirement, instead, is a topological one and can be reformulated in weaker ways. For example if the Hilbert space is separable one only needs to require that for all \( \psi, \phi \in \mathcal{H} \) the function \( t \to \langle U(t)\psi, \phi \rangle \) is Lebesgue measurable. Unitary groups are uniquely determined by self-adjoint operators; this is the content of the Stone theorem, which we are going to discuss.

Given a unitary group, the operator \( A \) defined by:

\[
D(A) = \left\{ \psi \in \mathcal{H} : \exists \lim_{h \to 0} \frac{U(h) - \mathbb{I}}{h} \psi \right\},
\]

\[A\xi := i \lim_{h \to 0} \frac{U(h) - \mathbb{I}}{h} \xi,\]

is called the infinitesimal generator of \( U(t) \), for which the following property holds:

\[
U(t)A\xi = AU(t)\xi \quad \forall \xi \in D(A), t \in \mathbb{R}.
\]

The parameter \( t \) when given the role of time plays an important part in the quantum mechanical description of physical systems since, in this case, the infinitesimal generator is the operator corresponding to the total energy of the system, which as we know, is the Hamiltonian. Besides, unitary groups on a Hilbert space can be considered, roughly speaking, as given by the exponentiation of certain self-adjoint operators. In fact given \( A \), a self-adjoint operator with its spectral measure \( E_{\lambda} \), by the functional calculus associated to the spectral theorem we define:

\[
e^{-itA} := \int_{\mathbb{R}} e^{-it\lambda} dE_{\lambda} \quad t \in \mathbb{R},\]

and prove that:

**Proposition 3.1.** Given \( A \) a self-adjoint operator, the family \( \{U(t) = e^{-itA} : t \in \mathbb{R}\} \) is a strongly continuous one-parameter group on \( \mathcal{H} \). Moreover, \( A \) is its infinitesimal generator, in the sense of (3.7) and (3.8).

In the most general situations it is difficult to write down explicit expressions for \( e^{-itA} \), nevertheless one can prove that every unitary group can be obtained by exponentiating a unique self-adjoint operator, namely its generator:

**Theorem 3.2.** (Stone’s theorem) If \( U \) is a strongly continuous one-parameter unitary group on \( \mathcal{H} \), then there exists a unique self-adjoint operator \( A \) such that \( U(t) = e^{-itA} \) for \( t \in \mathbb{R} \).
There is a very useful corollary of the Stone theorem, but we need the notion of core of an operator.

From the general theory of operators on a Hilbert space. Given an operator $B$, a linear subspace of $D(B)$, say $\mathcal{D}$, is a core for $B$ if $\mathcal{D}$ is dense in $(D(B), \| \cdot \|_B)$. If $B$ is a closed operator, a linear subspace $\mathcal{D}$ of $D(B)$ is a core for $B$ if and only if $B$ is the closure of its restriction on $\mathcal{D}$. A closed operator, then, can be obtained from its restriction to any core. In fact, as we are going to explicitly check in the case of the generators of translations and dilations, sometimes closed operators are more easily handled on some suitable core rather than on their full domains.

From the Stone theorem, it follows that:

**Corollary 3.3.** Let $T$ be a self-adjoint operator and the infinitesimal generator of the unitary evolution group $U(t)$. If $\mathcal{D}$ is a dense subspace of $D(T)$ and $U(\mathcal{D}) \subset \mathcal{D}$ then $\mathcal{D}$ is a core for $T$.

The above theorem, along with its corollary, is a cornerstone in functional analysis and we are now going to use them in order to explicitly study the unitary groups of translations and dilations.

### 3.2.1 The Unitary Group of Translations

We focus on the unitary group of space translations lifted on $\mathcal{H} = L^2(\mathbb{R})$ and we are going to prove that its infinitesimal generator is the momentum operator:

$$ p : D(p) = H^1(\mathbb{R}) \to \mathcal{H}, \quad p\psi = -i\psi'. \quad (3.11) $$

Spatial translations are implemented by:

$$ (T(a)\psi)(x) = \psi(x - a), \quad (3.12) $$

ad since Lebesgue measure is translational invariant it is straightforward to prove that $\{T(a)\}_{a \in \mathbb{R}}$ form a one-parameter group.

Moreover if $\psi, \phi \in C^\infty_0(\mathbb{R})$ one can prove by dominated convergence that:

$$ \langle T(a)\psi, \phi \rangle = \int_\mathbb{R} \overline{\psi(x - a)} \phi(x) \xrightarrow{a \to 0} \langle \psi, \phi \rangle, \quad (3.13) $$
and since \(C_0^\infty(\mathbb{R})\) is dense in \(L^2(\mathbb{R})\) then \(T(a)\) is weakly (and then strongly) continuous over the whole Hilbert space. From Stone’s theorem its infinitesimal generator is a self-adjoint operator, that we now compute.

Let \(\psi \in C_0^\infty(\mathbb{R})\) and consider:

\[
i (T(a) - I) \psi(x) = i (\psi(x - a) - \psi(x)) = -i \int_{x-a}^x \psi'(s) ds,
\]

(3.14)

and if we take \(|a| \leq 1\) we get:

\[
\left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| \leq \frac{1}{a} \int_{x-a}^x |\psi'(x) - \psi'(s)| ds.
\]

(3.15)

Moreover since \(\psi'\) is continuous, we have:

\[
\frac{1}{a} \int_{x-a}^x |\psi'(x) - \psi'(s)| ds \leq \max_{s \in [x-a, x]} |\psi'(x) - \psi'(s)| \to 0, \quad a \to 0,
\]

(3.16)

which means that:

\[
\left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| \to 0.
\]

(3.17)

In order to extend this notion of convergence to \(L^2(\mathbb{R})\) we need to make use of the theorem of dominated convergence, that is we need to determine a function \(g \in L^1(\mathbb{R})\) such that:

\[
\left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| \leq g(x) \quad \forall a, \, |a| \leq 1.
\]

(3.18)

From (3.15) we infer that:

\[
\left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| \leq \frac{1}{a} \int_{x-a}^x |\psi'(x)| + |\psi'(s)| ds \leq 2 \|\psi'\|_\infty \chi_S \in L^1(\mathbb{R}).
\]

(3.19)

A few words on \(S\) are in need. Of course we can write:

\[
\left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| = \left| \frac{i}{a} T(a) - I \psi(x) + i \psi'(x) \right| \chi_S(x),
\]

(3.20)

where \(S\) is the support of the function in the argument of the module, that is:

\[
S \subset \text{supp } \psi \cup \bigcup_{a \in [0,1]} \text{supp } (T(a)\psi) = \bigcup_{a \in [0,1]} \text{supp } (T(a)\psi),
\]

(3.21)
because \( \text{supp } \psi' \subset \text{supp } \psi \) and \( \text{supp } \psi = \text{supp } (T(0)\psi) \). Moreover, since \( \text{supp } (T(a)\psi) = (\text{supp } \psi) + a \) and \( a \in [0,1] \), compact subset in \( \mathbb{R} \), we have that:

\[
\bigcup_{a \in [0,1]} \text{supp } (T(a)\psi) = \bigcup_{a \in [0,1]} (\text{supp } \psi + a) = \{ x + a : x \in \text{supp } \psi, a \in [0,1] \}, \quad (3.22)
\]

so that \( S \) is a subset of a compact real interval:

\[
|x + a| \leq |x| + |a| \Rightarrow \text{diam } \{ x + a | x \in \text{supp } \psi, a \in [0,1] \} \leq \text{diam } (\text{supp } \psi) + 1. \quad (3.23)
\]

Given \( \psi \in C^\infty_0(\mathbb{R}) \) one has that:

\[
\left\| \frac{i}{a} T(a) - \frac{1}{a} \psi + i\psi' \right\|_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \left| \frac{1}{a} (T(a) - I) \psi(x) + i \psi'(x) \right|^2 \, dx. \quad (3.24)
\]

Then, by dominated convergence we obtain that:

\[
\left\| \frac{i}{h} T(a) - \frac{1}{h} \psi + i\psi' \right\|_{L^2(\mathbb{R})} \to 0 \quad \forall \psi \in C^\infty_0(\mathbb{R}). \quad (3.25)
\]

Thus the generator \( A \) acts as the momentum operator on the space of test functions:

\[
A|_{C^\infty_0(\mathbb{R})} = p|_{C^\infty_0(\mathbb{R})}. \quad (3.26)
\]

Since \( T(a)C^\infty_0(\mathbb{R}) \subset C^\infty_0(\mathbb{R}) \), from Corollary (3.3) it follows that \( C^\infty_0(\mathbb{R}) \) is a core for the generator \( A \), that is:

\[
A = \overline{A} = \overline{A|_{C^\infty_0(\mathbb{R})}}. \quad (3.27)
\]

Thus, we can infer that:

\[
A = \overline{A|_{C^\infty_0(\mathbb{R})}} = \overline{p|_{C^\infty_0(\mathbb{R})}} = p, \quad (3.28)
\]

and by the Stone Theorem we have:

\[
T(a) = \exp (-ia \, p) \quad \forall a \in \mathbb{R}. \quad (3.29)
\]

From the explicit expression in (3.12) it is easy to understand why \( T(a) \) is said to generate translations on the Hilbert space: after the action of \( T(a) \), the whole function is rigidly moved of a fixed quantity \( a \) (Figure 3.3). With such an in-
interpretation it is easier to understand the different self-adjoint extensions of the operator $p$ over both bounded and unbounded intervals in $\mathbb{R}$.

If we consider the whole real line one can freely translate functions to both sides so that the generator of translations is well defined and $p$ is essentially self-adjoint. In this thesis we are more interested in the case of bounded intervals, where one can translate the functions up to an end and needs to give a prescription on how it comes back in the interval from the other end in order to preserve unitarity. Wave functions can come back in with a different fixed phase, and each of them corresponds to a different self-adjoint extension of $p$.

Similarly for the momentum on a half line we can freely translate functions in one direction, however what reaches the origin cannot enter at the other end since it is located at infinity. Thus the momentum on an half-line cannot be an observable.

### 3.2.2 The Unitary Group of Dilations

Similarly we can compute the explicit expression of the infinitesimal generator of the dilation unitary group. We start with:

$$\left( D(s) \psi \right)(x) = e^{-s/2} \psi(e^{-s}x),$$

(3.30)

and prove that $\{D(s)\}_{s \in \mathbb{R}}$ is a strongly continuous unitary group and that its infinitesimal generator is given by the virial operator over its maximal domain.

It is easy to check that $\{D(s)\}_{s \in \mathbb{R}}$ is a unitary group; we now prove it is continuous. First, we take $\phi \in C_0^\infty(\mathbb{R})$, which, as in the case of translations, is a core for the
virial operator, and compute:

$$\langle \phi, D(h)\phi \rangle = \int_\mathbb{R} \bar{\phi}(x)e^{-h/2}\phi(e^{-h}x)dx. \quad (3.31)$$

Then, if we consider $0 \leq h/2 \leq 1$:

$$|\bar{\phi}(x)e^{-h/2}\phi(e^{-h}x)| \leq \|\phi\|_\infty e^{-h/2} |\phi(x)| \leq e \|\phi\|_\infty |\phi(x)| \in L^1(\mathbb{R}), \quad (3.32)$$

so that, by dominated convergence:

$$\langle \phi, D(h)\phi \rangle \underset{h \to 0}{\longrightarrow} \langle \phi, \phi \rangle \quad \forall \phi \in C^\infty_0(\mathbb{R}). \quad (3.33)$$

Then, one can extend by density this convergence up to the whole Hilbert space because $C^\infty_0(\mathbb{R})$ is dense in $L^2(\mathbb{R})$.

By the polarization identity it follows that:

$$\langle \phi, D(h)\psi \rangle \underset{h \to 0}{\longrightarrow} \langle \phi, \psi \rangle \quad \forall \phi, \psi \in L^2(\mathbb{R}), \quad (3.34)$$

which means that $\{D(s)\}_{s \in \mathbb{R}}$ is weakly continuous, and from this, it follows that it is strongly continuous as well.

We, now, investigate the nature of its generator. First we fix $\phi \in C^\infty_0(\mathbb{R})$ and compute:

$$\frac{i}{s}(D(s) - I)\phi(x) = i \left( \frac{e^{-s/2}\phi(e^{-s}x) - \phi(x)}{s} \right). \quad (3.35)$$

This sequence converges pointwise to:

$$i \left( \frac{e^{-s/2}\phi(e^{-s}x) - \phi(x)}{s} \right) \underset{s \to 0}{\longrightarrow} i \left( \frac{d}{ds}e^{-s/2}\phi(e^{-s}x) \right)_{s=0} = (xp - \frac{i}{2})\phi(x), \quad (3.36)$$

with $p$ the momentum operator. Once more we need to extend the previous pointwise convergence to $L^2(\mathbb{R})$, which can be carried out by the dominated convergence theorem, as for the case of translations.

We start observing that:

$$i \frac{e^{-s/2}\phi(e^{-s}x) - \phi(x)}{s} = i \frac{1}{s} \int_0^s \frac{d}{dt}(e^{-t/2}\phi(e^{-t}x)) \ dt, \quad (3.37)$$
and look for a function \( g \in L^1(\mathbb{R}) \) such that

\[
\left| \frac{i}{s} (D(s) - I) \phi(x) - \left( xp - \frac{i}{2} \right) \phi(x) \right| \leq g(x) \quad \forall s, |s| \leq 1.
\]  (3.38)

Once proved that, by the dominated convergence theorem it follows that \( \forall \phi \in C_0^\infty(\mathbb{R}) \):

\[
\left\| \frac{i}{s} (D(s) - I) \phi - \left( xp - \frac{i}{2} \right) \phi \right\|_{L^2(\mathbb{R})} \xrightarrow{s \to 0} 0.
\]  (3.39)

We now prove this. Take:

\[
\left| \frac{i}{s} (D(s) - I) \phi(x) + i \left( x\phi' + \frac{1}{2} \phi(x) \right) \right| =
\leq \frac{1}{s} \int_0^s \left[ \frac{d}{dt} \left( e^{-t/2} \phi(e^{-t}x) \right) - \left( \frac{d}{dt} \left( e^{-t/2} \phi(e^{-t}x) \right) \right)_{t=0} \right] dt \leq
\leq 2 \left\| \frac{d}{dt} e^{-t/2} \phi(e^{-t}x) \right\|_\infty \chi_S(x),
\]  (3.40)

where \( S \), is a subset of the following union:

\[
S \subset \supp \phi \bigcup_{s \in [0,1]} \supp (D(s)\phi) \cup \supp (x\phi') = \bigcup_{s \in [0,1]} \supp (D(s)\phi).
\]  (3.41)

Since \( \supp (D(s)\phi(x)) = e^s \supp \phi(x) \) and \( s \in [0,1] \), then:

\[
S \subset \bigcup_{s \in [0,1]} \supp (D(s)\phi) = e \supp \phi(x).
\]  (3.42)

As in the case of the translation group we can use the dominated convergence, so that \( (3.39) \) holds \( \forall \phi \in C_0^\infty(\mathbb{R}) \). Moreover, it is straightforward to check, by the corollary of the Stone theorem, that \( C_0^\infty(\mathbb{R}) \) is a core for the generator of the dilation group.

So far we have proved for the generator \( T \) that:

- \( T|_{C_0^\infty(\mathbb{R})} = -i \left( x \frac{d}{dx} + \frac{1}{2} \right) \),
- \( C_0^\infty(\mathbb{R}) \) is a core for \( T \).
Then, we infer that:

\[ T = T|_{C^\infty_0(\mathbb{R})} = -i \left( x \frac{d}{dx} + \frac{1}{2} \right), \quad (3.43) \]
\[ D(T) = \{ \psi \in L^2(\mathbb{R}) \mid x\psi' \in L^2(\mathbb{R}) \}, \quad (3.44) \]

and, in the end, we get the final expression for the generator:

\[ T = xp - \frac{i}{2}. \quad (3.45) \]

Before moving on and leaving the group of dilations we now want to prove that the generator of this group is exactly the \textit{virial} operator.

Let \( \phi \) be an element in \( C^\infty_0(\mathbb{R}) \), so the following equality holds:

\[ -i \left( x \frac{d}{dx} + \frac{1}{2} \right) \phi(x) = -\frac{i}{2} \left( x \frac{d}{dx} \phi(x) + \frac{d}{dx} (x\phi(x)) \right). \quad (3.46) \]

Following the same path and using the uniqueness of the closure we obtain that:

\[ T = xp - \frac{i}{2} = \frac{1}{2} (xp + px) =: x \circ p. \quad (3.47) \]

So that, by the Stone theorem:

\[ D(s) = \exp \left( -i s (x \circ p) \right). \quad (3.48) \]
Chapter 3. Moving Walls and Geometric Phases

3.2.3 The DilaTranslation

In the previous sections, we showed a way of lifting translations and dilations over $L^2(\mathbb{R})$. A composition of a translation and a dilation can map our initial problem (3.3) into an easier one. This is the core of this section, but before that, we prove an identity that will be useful further on:

\[ D^*(\ln l)pD(\ln l) = \frac{p}{l}, \quad l > 0. \] (3.49)

Let us define:

\[ p(s) = D^*(s)pD(s), \] (3.50)

and if we compute its derivative with respect to the parameter $s$ we obtain:

\[ \frac{d}{ds}p(s) = i[x \circ p, p(s)] = iD^*(s)[x \circ p, p]D(s) = -D^*(s)pD(s) = -p(s), \] (3.51)

since $[x \circ p, p] = ip$ and $[x \circ p, D(s)] = 0 = [x \circ p, D^*(s)]$.

Equation (3.51) admits one and only one solution given the initial condition $p(s = 0) = p$, that is:

\[ p(s) = e^{-sp}. \] (3.52)

Thus, if we plug $s = \ln l$ into equation (3.52) we get (3.49).

Next, we consider the family of unitary operators, which is given by a well-defined composition of (3.6):

\[ U(l,a) : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \quad U(l,a) = D^*(\ln l)T^*(a), \] (3.53)

We need to remark that the two-parameter family we have built up does not form a group.

We are mapping $H(l,a)$ into:

\[ H(l) = U(l,a)H(l,a)U^*(l,a), \] (3.54)

whose transformed domain, is \textit{time independent} and reads

\[ D(H(l)) = D \oplus L^2(I^c), \] (3.55)
where $I^c$ is the complementary set of $I = [-\frac{1}{2}, \frac{1}{2}]$ and $D = U(l, a)D_{l,a}$ is given by

$$D \equiv \left\{ \psi \in \mathcal{H}^2(I) : \psi\left(-\frac{1}{2}\right) = \eta \psi\left(\frac{1}{2}\right), \quad \bar{\eta} \psi'\left(-\frac{1}{2}\right) = \psi'\left(\frac{1}{2}\right) \right\}. \quad (3.56)$$

We have thus achieved one of our goals, that is map our initial family of Hamiltonians with time-dependent domains into a family with a common fixed domain of self-adjointness. This has been possible thanks to the dilatranslation and, most importantly, to the choice of boundary conditions as discussed in 2.5.1. We have taken into account those boundary conditions which do not mix derivatives and functions at the border; these are the only ones which leave the transformed domain $U(l, a)D_{l,a}$ time-independent. In fact, if any explicit temporal dependence occurs, it cancels out identically due to equation (2.43), which do not mix functions with their derivatives. For example, if an expression like:

$$\psi\left(a - \frac{l}{2}\right) + \psi'\left(a + \frac{l}{2}\right) = 0, \quad (3.57)$$

had appeared in $D_{l,a}$, then after the dilatranslation in (3.53) and due to (3.49) we would have obtained:

$$\psi\left(\frac{1}{2}\right) + \frac{1}{l} \psi'\left(\frac{1}{2}\right) = 0, \quad (3.58)$$

which is of course time dependent for the $l$ in the denominator.

As we are going to prove in the next section, it is easier to study the spectral decomposition of $H(l)$, since:

$$H(l) = U(l, a)H(l, a)U^*(l, a) = \frac{1}{l^2} \frac{p^2}{2m} \oplus 0 = -\frac{1}{l^2} \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \oplus 0. \quad (3.59)$$

### 3.3 The Spectral Decomposition

Let us consider the following fixed-domain family of Hamiltonians:

$$H(l) = \frac{1}{l^2} \frac{p^2}{2m} \oplus 0, \quad (3.60)$$

and let:

$$D \equiv \left\{ \psi \in \mathcal{H}^2(I) : \psi\left(-\frac{1}{2}\right) = \eta \psi\left(\frac{1}{2}\right), \quad \bar{\eta} \psi'\left(-\frac{1}{2}\right) = \psi'\left(\frac{1}{2}\right) \right\}. \quad (3.61)$$
be the domain of the first member of the direct sum.

It will be shown that its spectral decomposition is in a one-to-one isometric correspondence with our initial problem and that the transformation, as already remarked, is implemented by a dilation and subsequently by a translation lifted on the Hilbert space.

Recalling that $p = -i \frac{d}{dx}$ we would like to solve the equation:

$$-\frac{1}{2m} \frac{d^2}{dx^2} \phi(x) = \lambda \phi(x),$$  \hspace{1cm} \text{(3.62)}

with the boundary conditions given by (3.61).

Of course what we are investigating is a particular case of a regular Sturm-Liouville problem [49], for which the following result holds:

**Theorem 3.4.** Let a regular Sturm-Liouville problem with boundary conditions provided by (3.61) be given.

1. All eigenvalues are real;

2. Eigenfunctions corresponding to distinct eigenvalues are orthogonal; that is if $f$ and $g$ are eigenfunctions with eigenvalues $\lambda \neq \mu$, then

$$\langle f, g \rangle = \int_I \overline{f(x)}g(x) \, dx = 0 \quad \text{(3.63)}$$

3. The eigenspace for any eigenvalue $\lambda$ is at most 2-dimensional. If the boundary conditions are separated, (that is each one involves a condition at only one endpoint), the eigenspace is always one dimensional.

Theorem [3.4] does not guarantee the existence of eigenfunctions for a regular Sturm-Liouville problem but rather shows some necessary conditions that eigenvalues and eigenfunctions must satisfy.

The following theorem bridges this gap:

**Theorem 3.5.** For the regular Sturm - Liouville problem (3.62) with boundary conditions given by (3.61) there is an orthonormal basis of $L^2(I)$ consisting of eigenfunctions.
Let us, now, solve equation (3.62).

From the theory of ordinary differential equations it is known that the general form of a solution is:

$$\phi(x) = A \cos(kx) + B \sin(kx) \quad A, B \in \mathbb{C} \quad k \in \mathbb{R}. \quad (3.64)$$

Substituting (3.64) in (3.62) we find the well known dispersion relation between energy and momentum:

$$\lambda = \frac{1}{2ml^2} k^2. \quad (3.65)$$

We would like to understand better the role played by the boundary conditions, which, as expected, will give rise to the quantization of the spectrum.

It is important to stress that the whole discussion lies on the choice of a particular set of boundary conditions, which have already been largely discussed in 2.5.1. If we impose that (3.64) belongs to $D$ and its norm being one we obtain that:

$$\phi(x) = \sin(kx) \pm e^{i\alpha} \cos(kx), \quad (3.66)$$

is a solution of the Sturm-Liouville problem (modulo an overall phase), provided that $\eta \neq \pm 1$.

The phase $\alpha$ is given by:

$$\alpha = \text{Arg}\left(\frac{1 + \eta}{1 - \eta}\right). \quad (3.67)$$

Moreover the quantization rule follows:

$$\tan\left(\frac{k}{2}\right) = \pm \left|\frac{1 - \eta}{1 + \eta}\right|. \quad (3.68)$$

Solving equation (3.68) in $k$:

$$k_n^{(\pm)} = \pm 2 \arctan\left|\frac{1 - \eta}{1 + \eta}\right| + 2n\pi, \quad n \in \mathbb{N}, \quad (3.69)$$

and plugging the result in (3.65) we easily find the discrete spectrum of the problem under analysis:

$$\lambda_n^{(\pm)} = \frac{2}{ml^2} \left(\pm \arctan\left|\frac{1 - \eta}{1 + \eta}\right| + n\pi\right)^2, \quad n \in \mathbb{N}. \quad (3.70)$$
We observe that if \( \eta \neq \pm 1 \) the spectrum is non-degenerate, that is, eigenfunctions and eigenvalues are in a one-to-one correspondence. In what follows we are going to use the notation \( k_n \equiv k^{(\pm)}_n \), which means that one eigenvalue with a definite sign has been selected.

As we are going to show, both cases with \( \eta = \pm 1 \) are degenerate. Let us start with \( \eta = 1 \).

In this case every function in the form (3.64) with \( k_n = 2n\pi \), \( n \in \mathbb{N} \) is an eigenfunction of our problem. It is interesting to observe that in the limit \( \eta \to 1 \) in equation (3.69) we recover the degenerate case from the non-degenerate one. The same will hold also in the case \( \eta \to -1 \). We have two free parameters \( A \) and \( B \) (module normalization of \( \phi \)), which means that for every \( n \in \mathbb{N} \) the corresponding eigenvalue determines a two-dimensional eigenspace.

An orthonormal basis in this space is given, for example, by:

\[
\begin{align*}
\phi^I(x) &= A \cos(k_n x) = A \cos(2\pi n x), \\
\phi^{II}(x) &= B \sin(k_n x) = B \sin(2\pi n x),
\end{align*}
\]

where \( A \) and \( B \) are such that \( |A|^2 = |B|^2 = 2 \) due to normalization and \( n \in \mathbb{N} \).

For instance, we could choose both \( A \) and \( B \) to equal \( \sqrt{2} \). The eigenvalues for \( \eta = 1 \) are:

\[ \lambda_n = \frac{2\pi^2}{ml^2} n^2 \quad n \in \mathbb{N}. \quad (3.72) \]

Similarly we can work out the case \( \eta = -1 \). Again, equation (3.64) represents an eigenfunction of our problem provided that \( k_n = (2n + 1)\pi \), \( n \in \mathbb{N} \) and once more we have a double degeneracy for every eigenvalue. An orthonormal basis in this space is given, for example, by:

\[
\begin{align*}
\phi^I(x) &= A \cos(k_n x) = A \cos((2n + 1)\pi x), \\
\phi^{II}(x) &= B \sin(k_n x) = B \sin((2n + 1)\pi x),
\end{align*}
\]

with \( |A|^2 = |B|^2 = 2 \). The eigenvalues for \( \eta = -1 \) are:

\[ \lambda_n = \frac{\pi^2}{2ml^2} (2n + 1)^2 \quad n \in \mathbb{N}. \quad (3.74) \]

Of course one might wonder whether the spectrum is only purely point or it has a continuous part. The following theorem will shed some light on this issue.
Theorem 3.6. Let $T : D(T) \subset \mathcal{H} \to \mathcal{H}$ be a symmetric operator on a separable Hilbert space $\mathcal{H}$. If $T$ has an orthonormal basis of eigenvectors, then $T$ is essentially self-adjoint and its spectrum, $\sigma(\bar{T})$, is the closure of the set of its eigenvalues.

If we apply the previous theorem to our self-adjoint Hamiltonian, we find that its spectrum (which of course is equal to the spectrum of its closure, since $H$ is self-adjoint and then closed), is the closure of the set of eigenvalues determined above in each separate case. The latter set is closed in the Euclidean topology of $\mathbb{C}$ because it is a countable union of isolated points. We have, therefore, proved that $H(l)$ has a purely point spectrum and determined its whole spectral decomposition. We are now going to return to (3.5) and determine its spectral decomposition.

Let $\xi$ be an arbitrary function belonging to $L^2(\mathbb{R} \setminus I)$; $\xi$ is clearly an eigenfunction of the $0$ operator on $L^2(\mathbb{R} \setminus I)$ with zero eigenvalue. Therefore we can extend $\phi_n$ to an eigenfunction of (3.5), $\phi_n \oplus \xi$, which can be chosen to be in $C^\infty_0(\mathbb{R})$. See below for an explicit construction.

Starting from the eigenvalue problem of $H(l)$ we can easily prove that:

\[
(U^*(l, a)(\phi_n \oplus \xi))(x) \equiv \phi_n(x; a, l) \oplus \xi(x; a, l) \equiv \psi_n(x; a, l),
\]

(3.75)

are eigenfunctions of (3.5) with the same eigenvalues of $H(l)$:

\[
H(l) \left( \phi_n \oplus \xi \right) = \lambda_n \left( \phi_n \oplus \xi \right);
\]

(3.76)

\[
\left( U(l, a) H(l, a) U^*(l, a) \right) \left( \phi_n \oplus \xi \right) = \lambda_n \left( \phi_n \oplus \xi \right);
\]

(3.77)

\[
H(l, a) \left( U^*(l, a) \left( \phi_n \oplus \xi \right) \right) = \lambda_n \left( U^*(l, a) \left( \phi_n \oplus \xi \right) \right),
\]

(3.78)

so that explicitly the transformed (back) eigenfunctions are:

\[
\psi_n(x; a, l) = \phi_n(x; a, l) \oplus \xi(x; a, l) = \frac{1}{\sqrt{l}} \phi_n \left( \frac{x-a}{l} \right) \oplus \xi \left( \frac{x-a}{l} \right).
\]

(3.79)

For example, in the case $\eta \neq \pm 1$ we explicitly have:

\[
\psi_n^{(\pm)}(x; a, l) = \frac{1}{\sqrt{l}} \left( \sin k_n^{(\pm)} \left( \frac{x-a}{l} \right) \pm e^{i\alpha} \cos k_n^{(\pm)} \left( \frac{x-a}{l} \right) \right) \oplus \xi \left( \frac{x-a}{l} \right).
\]

(3.80)
We would like to stress that since we started with eigenfunctions in $C^\infty(\mathbb{R})$ (that is $\phi_n \oplus \xi$) through the action of $U(l, a)$ we again obtained $C^\infty(\mathbb{R})$ eigenfunctions, and in addition these latter are naturally regular in the parameters $(a, l)$ domain.

Let us now exhibit an explicit construction of $\psi_n(x; a, l)$. For definiteness, we consider, first, the case $\eta \neq \pm 1$, that is the nondegenerate one. In light of the previous discussion we choose the following eigenfunctions for the Hamiltonian (3.5):

$$\psi_n(x; a, l) = \phi_n(x; a, l) \xi_\epsilon(x; a, l),$$  \hspace{1cm} (3.81)

where $\phi_n(x; a, l)$ are the eigenfunctions belonging to $D_{l,a} \subset L^2(I_{l,a})$ and determining the resolution of identity for the operator defined in (3.2) and (3.3); the $\xi_\epsilon(x)$ is, instead, a $C^\infty_c(\mathbb{R})$ function, such that it is constant on the interval $I_{l,a}$ and identically vanishes on $(-\infty, a - l/2 - \epsilon) \cup [a + l/2 + \epsilon, \infty)$.

We do not require any particular functional form in $[a - l/2 - \epsilon, a - l/2] \cup [a + l/2, a + l/2 + \epsilon]$ apart from smoothness up to the border. To be more precise we need to consider the analytical continuation of $\phi_n(x; a, l)$ over the whole real line, so that the product in (3.81) is well-posed. Of course, it will not belong to $L^2(\mathbb{R})$, but this will not alter the desired regularity property and integrability condition of $\phi_n(x; a, l) \xi_\epsilon(x; a, l)$.

This is a very specific prescription we are giving in order to tackle calculations involving derivatives of maps (such as $\phi_n(x; a, l)$) which are strictly confined in some intervals.

If we did not care about giving a regularization procedure and tried to compute the derivatives in the 1-form (see next section) without the introduction of the regularizer $\xi_\epsilon$, divergent contributions would naturally arise from the boundary.

In this renormalization scheme we are at first artificially embedding $L^2(I_{l,a})$ into $L^2(\mathbb{R})$ and then “mollifying” the boundary contribution through the introduction of the regularizer.

Finally, in the limit $\epsilon \to 0$ we make our way back to our initial problem.

We would like to stress, once more, that (3.81) is still an eigenfunction of (3.5) since $\phi_n(x; a, l)$ is an eigenfunction of the Hamiltonian (3.2) defined in (3.3) and $\psi_n|_{\mathbb{R} \setminus I_{l,a}}$ is an eigenfunction of the 0 operator with null eigenvalue.
3.4 The Abelian Phase: The Nondegenerate Case

In this section we are going to use the following notation:

\[
\psi_n(x; a, l) = \phi_n(x; a, l) \xi_e(x; a, l) \equiv \psi_n(x).
\]  

We would like to show the existence of a geometric phase in our problem through the evaluation of the following 1-form:

\[
\langle \psi_n, d\psi_n \rangle = \int_{\mathbb{R}} \psi_n(x)(d\psi_n)(x)dx.
\]  

It is important to stress that the exterior differential has to be defined over the parameter manifold and not on the coordinate domain of the eigenfunctions, that is:

\[
(d\psi_n)(x) = \left( \frac{\partial}{\partial l} \psi_n \right)(x)dl + \left( \frac{\partial}{\partial a} \psi_n \right)(x)da.
\]  

So that:

\[
\langle \psi_n, d\psi_n \rangle = \int_{\mathbb{R}} \psi_n(x) \frac{\partial}{\partial l} \psi_n(x)dx dl + \int_{\mathbb{R}} \psi_n(x) \frac{\partial}{\partial a} \psi_n(x)dx da.
\]  

Furthermore, we need to normalize (3.81), that is:

\[
\int_{\mathbb{R}} |\psi_n|^2 dx = 1.
\]  

We will show that, as stated in a broader theoretical framework (1.47), the 1-form defined above is purely imaginary. If we consider, for example, the first coefficient of the 1-form it is easy to prove that:

\[
\int_{\mathbb{R}} \psi_n \frac{\partial}{\partial l} \psi_n dx = \frac{1}{2} \int_{\mathbb{R}} \frac{\partial}{\partial l} |\psi_n|^2 dx + i \text{ Im} \int_{\mathbb{R}} \left( \frac{\phi_n}{\partial l} \phi_n \right) \xi_e^2 dx.
\]  

And analogously for the second coefficient we have:

\[
\int_{\mathbb{R}} \psi_n \frac{\partial}{\partial a} \psi_n dx = \frac{1}{2} \int_{\mathbb{R}} \frac{\partial}{\partial a} |\psi_n|^2 dx + i \text{ Im} \int_{\mathbb{R}} \left( \frac{\phi_n}{\partial a} \phi_n \right) \xi_e^2 dx.
\]
Plugging the explicit expressions of the eigenfunctions we find that:

\[
\text{Im} \int_{\mathbb{R}} \left( \phi_n \frac{\partial}{\partial l} \phi_n \right) \xi^2 \epsilon \, dx = \frac{k_n}{l^3} \sin \alpha \int_{\mathbb{R}} (x - a) \xi^2(x) \, dx,
\]

\[
\text{Im} \int_{\mathbb{R}} \left( \phi_n \frac{\partial}{\partial a} \phi_n \right) \xi^2 \epsilon \, dx = \frac{k_n}{l^2} \sin \alpha \int_{\mathbb{R}} \xi^2(x) \, dx.
\]

We are interested in the limit \( \epsilon \to 0 \), that is, by dominated convergence,

\[
\lim_{\epsilon \to 0} \int_{\mathbb{R}} \xi^2(x) \, dx = \int_{\mathbb{R}} \chi_{[a - \frac{l}{2}, a + \frac{l}{2}]}(x) \, dx = l,
\]

\[
\lim_{\epsilon \to 0} \int_{\mathbb{R}} (x - a) \xi^2(x) \, dx = \int_{\mathbb{R}} (x - a) \chi_{[a - \frac{l}{2}, a + \frac{l}{2}]}(x) \, dx = 0.
\]

It is essential to prove that under our hypotheses it is plausible to pull the derivative in (3.87) and (3.88) out of the integral sign, so that for fixed \( \epsilon \):

\[
\int_{\mathbb{R}} \frac{\partial}{\partial l} |\psi_n|^2 \, dx = \frac{\partial}{\partial l} \int_{\mathbb{R}} |\psi_n|^2 \, dx = 0,
\]

\[
\int_{\mathbb{R}} \frac{\partial}{\partial a} |\psi_n|^2 \, dx = \frac{\partial}{\partial a} \int_{\mathbb{R}} |\psi_n|^2 \, dx = 0.
\]

This can be easily done by noting that \( \psi_n \) has inherited from \( U^*(l, a) \) the right regularity properties in order to exchange the derivative with the integral sign.

We are now ready to write the final expression of the 1-form defined above:

\[
\langle \psi_n, d\psi_n \rangle = i \left( \frac{k_n}{l} \sin \alpha \right) \, da,
\]

(3.92)
where in the limit $\epsilon \to 0$ the eigenfunctions become: $\psi_n(x) = \phi_n(x) \chi_{[a - \frac{1}{2}, a + \frac{1}{2}]}(x)$. The 1-form obtained is manifestly not closed, so that it yields a nontrivial Abelian phase, which will be dependent on the integration path.

For definiteness we choose a rectangular path $C$ in the $l - a$ plane, as shown in Figure 3.5 and compute:

$$\Phi_n = \oint_C A^{(n)} = i \oint_C \langle \psi_n, d\psi_n \rangle, \quad (3.93)$$

whose only non-trivial contributions are given by the vertical components of the circuit.

The final result is:

$$\Phi_n = \oint_C A^{(n)} = k_n \left( \frac{1}{l_1} - \frac{1}{l_2} \right) (a_2 - a_1) \sin \alpha, \quad (3.94)$$

which, as expected, depends on the particular path chosen, on the energy eigenvalue unambiguously determined by $k_n$ and on the boundary conditions ($\sin \alpha$). In the spirit of the previous physical interpretations of our problem, as already
discussed in section 2.6 and shown in Figure 2.4 our cyclic adiabatic evolution could be thought as in Figure 3.6.

The Berry curvature $\mathcal{F}^{(n)}$ corresponding to the $n$-th spectral bundle, discussed in section 2.4 reads from equation (1.51):

$$\mathcal{F}^{(n)} = dA^{(n)} = d\left(-\frac{k_n}{l} \sin \alpha \, da\right) = -k_n \sin \alpha \, d\left(\frac{1}{l} \, da\right) = \frac{k_n}{l^2} \sin \alpha \, dl \wedge da.$$  

(3.95)

The above equation brings to mind the curvature of a hyperbolic Riemannian manifold. Indeed, consider the Poincaré half-plane, which by definition is the upper-half plane together with the Poincaré metric:

$$ds^2 = \frac{dx^2 + dy^2}{y^2}.$$  

(3.96)

This half-plane is a model of hyperbolic geometry, whose geodesics are depicted in Figure 3.7. Then if we consider the Ricci tensor the only non vanishing components are:

$$R_{11} = R_{22} = -\frac{1}{y^2},$$  

(3.97)

which have the same structure as the Berry curvature (3.95) of our quantum mechanical model.
3.4.1 Another perspective for the same view

One may object the latter machinery for its artificiality, since, in order to regularize our boundary problem, we need to embed it into $\mathbb{R}$, that is into a fictitious larger space.

Physically, in fact, we can have access only on the inside of our box $I_{t,a}$, in other words we would like to find a way of performing the latter computations intrinsically, without introducing arbitrary larger spaces.

Another drawback may be the arbitrariness which lies underneath the choice of the embedding procedure; the one we made in (3.5) is no special, rather, it was chosen for the sake of simplicity.

Instead of forcing an embedding of $L^2(I_{t,a})$ into $L^2(\mathbb{R})$, let us now consider $L^2(I_{t,a})$ as the Hilbert space we are interested in. Again, we can trace back the path taken above and we would like to make sense of $\partial_a \phi_n(x; a, l)$. We know that $\phi_n(x; a, l) \in L^2(I_{t,a}) \subset L^1_{\text{loc}}(I_{t,a})$ so that we can uniquely identify it with a suitable distribution and, chosen $C^\infty_0(\Hat{I}_{t,a})$ as the space of test functions on the open interval $\Hat{I}_{t,a}$, we can consider its distributional derivative, with respect, for example, to the parameter $a$. Thus, we can start from the functional:

$$\xi \in C^\infty_0(\Hat{I}_{t,a}) \rightarrow \langle \phi_n(x; a, l), \xi \rangle \in \mathbb{C} \quad \phi_n(x; a, l) \in D_{t,a},$$

and try to make sense of the distributional derivative (with respect to the parameter $a$):

$$\xi \in C^\infty_0(\Hat{I}_{t,a}) \rightarrow \langle \partial_a \phi_n(x; a, l), \xi \rangle = ?$$

From the explicit expression of the solutions, compare with equation (3.79), we know that:

$$\phi_n(x; a, l) = \frac{1}{\sqrt{l}} \phi_n \left( \frac{x - l a}{a} \right) \quad \phi_n \in C^\infty(\mathbb{R}),$$

so that we can use integration by parts and obtain:

$$\int_{\Hat{I}_{t,a}} \frac{1}{\partial_a \sqrt{l}} \phi_n \left( \frac{x - l a}{a} \right) \xi(x) dx = \int_{\Hat{I}_{t,a}} \frac{1}{\sqrt{l}} \left( \frac{\partial}{\partial x} \phi_n \right) \left( \frac{x - a}{l} \right) \left( - \frac{1}{l} \right) \xi(x) dx$$

$$= - \int_{\Hat{I}_{t,a}} \frac{1}{\sqrt{l}} \left( \frac{1}{l} \right) \phi_n \left( \frac{x - a}{l} \right) \frac{\partial}{\partial x} \xi(x) dx.$$
We recall that a distribution $T$ is said to be regular if there exists a locally integrable function $f$ on $\Omega$ (nonempty open subset in $\mathbb{R}$) such that:

$$T(\phi) = \int_{\Omega} f(x)\phi(x)dx \quad \forall \phi \in C_0^\infty(\Omega).$$  \hfill (3.102)

The importance of regular distributions relies on the possibility of identifying them with locally summable functions. From (3.101) we can identify the above defined distributional derivative with a locally summable function on $\mathring{\mathcal{I}}_{l,a}$, that is $\partial_{l,a}\phi_n(x; a, l)$ restricted to $\mathring{\mathcal{I}}_{l,a}$ which belongs to $L^1_{\text{loc}}(\mathring{\mathcal{I}}_{l,a}) \supset L^2_{\text{loc}}(\mathring{\mathcal{I}}_{l,a})$ so that it defines uniquely the regular distribution above. Of course the same can be done for $\partial_{l}\phi_n(x; a, l)$. Doing so we are defining a way to calculate the 1-form coefficients in order to get rid of divergent contributions arising from the boundary.

Let us return to our problem settled in $\mathcal{H} = L^2(\mathring{\mathcal{I}}_{l,a})$. This time the 1-form expression is given by:

$$\langle \phi_n, d\phi_n \rangle = \left( \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \left( \frac{\partial}{\partial l} \phi_n \right)(x)dx \right)dl + \left( \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \left( \frac{\partial}{\partial a} \phi_n \right)(x)dx \right)da,$$  \hfill (3.103)

where the derivatives in (3.103) are to be considered in the prescription presented above, that is locally integrable functions in $\mathring{\mathcal{I}}_{l,a}$. Once more:

$$\int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial l} \phi_n(x)dx = \int_{\mathring{\mathcal{I}}_{l,a}} \frac{\partial}{\partial l} |\phi_n(x)|^2 dx - \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial l} \phi_n(x)dx. \hfill (3.104)$$

Due to normalization the first factor in the second member vanishes so that:

$$\text{Re} \left( \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial l} \phi_n(x)dx \right) = 0,$$  \hfill (3.105)

and as seen before (3.90):

$$\int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial l} \phi_n(x)dx = i \text{ Im} \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial l} \phi_n(x)dx. \hfill (3.106)$$

Following the same procedure we also obtain:

$$\int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial a} \phi_n(x)dx = i \text{ Im} \int_{\mathring{\mathcal{I}}_{l,a}} \phi_n(x) \frac{\partial}{\partial a} \phi_n(x)dx. \hfill (3.107)$$

With this in mind we are able to reach the boundary from the inside, rather than from the “outside”, so that our new prescription, though equivalent to the one
already discussed, may appear more natural.

So far we have considered the non-degenerate case and in particular the solutions with “+ sign” in (3.66). Analogous calculations can be computed for the symmetric case. Let us now move on to the \( \eta = \pm 1 \) cases.

### 3.5 The Degenerate Case

From the general theory of geometric phases it is well known that a degenerate spectral decomposition gives rise to a one form connection in terms of a Hermitian matrix and from a geometrical perspective this corresponds to a principal bundle, whose typical fiber is identified with a non-Abelian group. This has already been discussed in section 1.6. Let us consider the case \( \eta = 1 \), which physically corresponds to periodic boundary conditions. In this particular case we are explicitly deforming the interval topology into the topology of a circle, since we are identifying the interval endpoints. (See Figure 3.8)
Briefly our data are:

\[
\begin{align*}
\phi_I^n(x) &= \frac{A}{\sqrt{l}} \cos \left( k_n \frac{x - a}{l} \right), \\
\phi_{II}^n(x) &= \frac{B}{\sqrt{l}} \sin \left( k_n \frac{x - a}{l} \right),
\end{align*}
\]

where \( k = 2n\pi, \ n \in \mathbb{N} \)

| \( A \) | \( B \) |
| 2 | 2 |

and we need to compute:

\[
\mathcal{A}^{(n)} = i \left( \langle \phi_I^n, d\phi_I^n \rangle \langle \phi_{II}^n, d\phi_{II}^n \rangle \langle \phi_{II}^n, d\phi_{II}^n \rangle \right),
\]

where the coefficients of the differentials in (3.109) are to be considered in the distributional sense, like we did in section 3.4.1. Of course (3.109) can be rewritten as:

\[
\mathcal{A}^{(n)} = \mathcal{A}_l^{(n)} dl + \mathcal{A}_a^{(n)} da,
\]

where:

\[
\begin{align*}
\mathcal{A}_l^{(n)} &= i \left( \langle \phi_I^n, \frac{\partial}{\partial l} \phi_I^n \rangle \langle \phi_{II}^n, \frac{\partial}{\partial l} \phi_{II}^n \rangle \langle \phi_{II}^n, \frac{\partial}{\partial l} \phi_{II}^n \rangle \right), \\
\mathcal{A}_a^{(n)} &= i \left( \langle \phi_I^n, \frac{\partial}{\partial a} \phi_I^n \rangle \langle \phi_{II}^n, \frac{\partial}{\partial a} \phi_{II}^n \rangle \langle \phi_{II}^n, \frac{\partial}{\partial a} \phi_{II}^n \rangle \right).
\end{align*}
\]

Let us consider the general term:

\[
\langle \phi_i^n, d\phi_j^n \rangle = \left( \int_{I_{l,a}} \overline{\phi_i^n(x)} \left( \frac{\partial}{\partial l} \phi_j^n \right)(x) dx \right) dl + \left( \int_{I_{l,a}} \overline{\phi_i^n(x)} \left( \frac{\partial}{\partial a} \phi_j^n \right)(x) dx \right) da,
\]

where \( i, j \in \{I, II\} \).

In particular for the diagonal terms we obtain once more:

\[
\begin{align*}
\int_{I_{l,a}} \overline{\phi_I^n(x)} \frac{\partial}{\partial l} \phi_I^n(x) dx &= i \text{ Im} \int_{I_{l,a}} \overline{\phi_I^n(x)} \frac{\partial}{\partial l} \phi_I^n(x) dx, \\
\int_{I_{l,a}} \overline{\phi_I^n(x)} \frac{\partial}{\partial a} \phi_I^n(x) dx &= i \text{ Im} \int_{I_{l,a}} \overline{\phi_I^n(x)} \frac{\partial}{\partial a} \phi_I^n(x) dx.
\end{align*}
\]

From the explicit expressions in (3.108) we easily find that:

\[
\langle \phi_I^n, d\phi_I^n \rangle = 0 = \langle \phi_{II}^n, d\phi_{II}^n \rangle,
\]

where the coefficients of the differentials in (3.109) are to be considered in the distributional sense, like we did in section 3.4.1. Of course (3.109) can be rewritten as:
that is to say the diagonal terms identically vanish.

We now investigate the off-diagonal terms:

\[
\int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial l} \phi_i^j(x) dx = \frac{1}{2} \int_{I_{t,a}} \left( \phi_i^j(x) \frac{\partial}{\partial l} \phi_i^j(x) - \phi_i^j(x) \frac{\partial}{\partial l} \phi_i^j(x) \right) dx, \tag{3.116}
\]

\[
\int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial a} \phi_i^j(x) dx = \frac{1}{2} \int_{I_{t,a}} \left( \phi_i^j(x) \frac{\partial}{\partial a} \phi_i^j(x) - \phi_i^j(x) \frac{\partial}{\partial a} \phi_i^j(x) \right) dx. \tag{3.117}
\]

For \( i = j \) we return to (3.113)-(3.114) and in addition, for both cases we have that:

\[
\int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial l} \phi_i^j(x) dx = - \int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial l} \phi_i^j(x) dx, \tag{3.118}
\]

\[
\int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial a} \phi_i^j(x) dx = - \int_{I_{t,a}} \phi_i^j(x) \frac{\partial}{\partial a} \phi_i^j(x) dx. \tag{3.119}
\]

showing that (3.109) is Hermitian. One then finds that:

\[
\mathcal{A}^{(n)} = \mathcal{A}_l^{(n)} dl + \mathcal{A}_a^{(n)} da = i \begin{pmatrix} 0 & -\frac{1}{2} \frac{ABk}{l} \\ \frac{1}{2} \frac{ABk}{l} & 0 \end{pmatrix} da, \tag{3.120}
\]

since \( \mathcal{A}_l^{(n)} \equiv 0 \) and, if we choose \( AB \in \mathbb{R} \), that is \( AB = 2 \), we then get:

\[
\mathcal{A}^{(n)} = \frac{k_n}{l} \sigma_2 da. \tag{3.121}
\]

where \( \sigma_2 \) is the second Pauli matrix. The result we found cannot be interpreted in terms of a pure non-Abelian phase, since if we compute the curvature associated to this vector-valued one-form it is given by the formula:

\[
\mathcal{F}^{(n)} = d\mathcal{A}^{(n)}, \tag{3.122}
\]

exactly like in the Abelian case. In fact, in general, for a non-Abelian principal fiber bundle, the curvature two-form, according to the Cartan structure equation (see equation (1.84)), is provided by:

\[
\mathcal{F}^{(n)} = d\mathcal{A}^{(n)} + \frac{1}{2} [\mathcal{A}^{(n)}, \mathcal{A}^{(n)}]. \tag{3.123}
\]

In our case, although every fiber in the bundle is bidimensional, it is a trivial bundle, and as stated above no non-Abelian contribution arises. The one-form
connection in equation (3.120) can, then, be *globally* diagonalized using a particular basis: the one provided by plane waves. Indeed, if we had started from a “rotated” basis, instead of (3.108):

\[
\phi^I_n(x) \pm i \phi^H_n(x) \propto e^{\pm ik_n x},
\]

(3.124)
due to Euler’s identity, and computed (3.120) in this new basis, we would have obtained a diagonal matrix. In the most general case, instead, one is able to determine only a *local* basis where the above one-form (3.120) is diagonal. In our case it is the globality that makes the difference, that is the triviality of the bundle.
Conclusions

The core topic of this thesis has been the discovery of a geometric phase in a given physical system: a quantum particle in a box with moving walls. This has been possible only after a thorough and systematic analysis of the possible boundary conditions which could be given to describe this physical situation.

We have understood how boundary conditions play a principal role in the study of precise physical situations, since they represent our link between the actual system and the mathematical model. In fact, we have been able to give a physical interpretation of boundary conditions based on scattering by plane waves, and understand their different physical interpretations.

The system under examination, though being characterized by a discrete spectrum, is described by an unbounded operator, and this has been a novelty, since in the most known applications of geometric phases, only bounded Hamiltonians are considered. This, of course, has needed some care in the calculations carried on, since divergent contributions could have easily arisen from the boundary, as largely discussed in the main text.

Further studies may involve a generalization to the case of a particle with a spin, that is an electron, confined in a box, and detect whether in that case as well, some phase may emerge. Mathematical difficulties may arise, since we would need to use spinor fields and it is seemingly possible that a further plausible renormalization prescription should be needed in the calculation of the one-form coefficients. It could be interesting, as well, to investigate more general kinds of boundary conditions in purely geometrical terms, and try to understand their subtle link with the phase discovered.

Moreover we have seen how non-Euclidean geometries may arise in the structure of the parameter manifold, unfolding, for sure, new geometrical ideas in the field.
Conclusions

of quantum mechanics. Framing quantum theories into a geometrical perspective is, needless to say, a fascinating and brave project both for theoretical reasons (as well as physically and philosophically speaking) and experimental ones.

It is surprising how for almost fifty years a fundamental part in the understanding of quantum mechanics had been completely overlooked, but since the veil had been lifted new horizons and thrilling perspectives are definitely ahead.

Let me end on a more cheerful note. The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. We should be grateful for it and hope that it will remain valid in future research and that it will extend, for better or for worse, to our pleasure even though perhaps also to our bafflement, to wide branches of learning.

E.P. Wigner [50]
Appendix A

Sobolev Spaces

La mesure de Dirac δ, introduite en mécanique ondulatoire sous le nom de fonction de Dirac, n’est pas une fonction.

L. Schwartz [51]

In the present work we make a massive use of Sobolev spaces, we now recall some basics definitions and results for these spaces following [52] and [53].

Sobolev spaces were introduced by S.L. Sobolev in order to study weak solutions of partial differential equations. The definitions on these spaces are intrinsically linked to the theory of distributions, whose legitimate father is Laurent Schwartz [51].

Sobolev had the same aim as Schwartz, that is, to generalize the notion of function and some classical operations on a larger set, where the Cauchy problem might have been easier to solve [54–56]. They both used the notion of convergence in function spaces and the method of generalizing functions and operations on them was basically the same. If on the one hand Sobolev’s theory helped him solving one specific problem (generalized solutions of differential equations) on the other, Schwartz developed a versatile theory, which tied together different trends in functional analysis, among which we recall:

- Heaviside’s operational calculus;
- generalized derivatives and generalized solutions to differential equations;
• improper functions (e.g. the \( \delta \) function).

Thus Sobolev invented distributions, but it was Schwartz who created the theory of distributions \[57\].

In the theory of Lebesgue integration one may be interested in identifying the class of functions which are primitives \[58\]. The class we are interested in is made up of the so called absolutely continuous (a.c.) functions. For a definition of a.c. functions see, for example, \[58]. Every a.c. function is continuous and has bounded variation. The importance of these functions lies in the following characterization theorem:

**Theorem A.1.** A function \( f \) in \([a,b]\) \((a,b \in \mathbb{R})\) is a.c. if and only if there is a function \( h \in L^1(a,b) \) such that:

\[
    f(x) - f(a) = \int_a^x h(t)\,dt \quad \text{for } x \in [a,b]. \tag{A.1}
\]

\( f \) is differentiable a.e. and \( f'(x) = h(x) \) a.e. in \([a,b]\).

Then one can introduce the Sobolev space \( \mathcal{H}^1(a,b) \) expressed in terms of absolutely continuous functions:

\[
    \mathcal{H}^1(a,b) = \{ f \in AC[a,b] : f' \in L^2(a,b) \}. \tag{A.2}
\]

There are some situations when, for example, we need to consider integrable functions over the whole real line so that we consider the following more general definition.

Let \( I = (a,b) \), which may be unbounded, and let \( p \) be a real number \( 1 \leq p \leq +\infty \). The Sobolev space \( W^{1,p}(I) \) is defined as:

\[
    W^{1,p}(I) = \left\{ u \in L^p(I) : \exists g \in L^p(I) \text{ s.t. } \int_I u\phi' = -\int_I g\phi \quad \forall \phi \in C_0^\infty(I) \right\} \tag{A.3}
\]

\[
    = \{ u \in L^p(I) : u' \in L^p(I) \} \tag{A.4}
\]

where with the symbol \( u' \) we mean the distributional derivative of \( u \). We define:

\[
    \mathcal{H}^1(I) = W^{1,2}(I) \tag{A.5}
\]

so that if \( I \) is bounded we find again \((A.2)\).

It is useful to remark that in the case \( u \in C^1(I) \cap L^p(I) \), \( u' \in L^p(I) \), here we...
are using the classical derivative of $u$, then $u \in W^{1,2}(I)$. If $I$ is bounded, then, $C^1(\overline{I}) \subset W^{1,p}(I)$.

Sobolev spaces can be equipped with the norm:

$$\|u\|_{W^{1,p}} = \|u\|_{L^p} + \|u'\|_{L^p},$$

which cannot be obtained from a scalar product. Instead, the space $H^1$ is equipped with the scalar product:

$$\langle u, v \rangle_{H^1} = \langle u, v \rangle_{L^2} + \langle u', v' \rangle_{L^2},$$

whose associated norm is:

$$\|u\|_{H^1} = \sqrt{\|u\|_{L^2}^2 + \|u'\|_{L^2}^2},$$

which is equivalent to (A.6) for $p = 2$. Provided these facts about the norms in these spaces, one can prove that:

**Proposition A.2.** The space $W^{1,p}$ is a Banach space for $1 \leq p \leq \infty$. It is reflexive for $1 < p < \infty$ and separable for $1 \leq p < \infty$. The space $H^1$ is a separable Hilbert space.

We finish this quick and partial summary about Sobolev spaces with a theorem and with the definition of $H^2$. Theorem A.3 states (roughly speaking) that the functions in $W^{1,p}$ are the primitives of $L^p$ functions:

**Theorem A.3.** Let $u \in W^{1,p}$, $1 \leq p \leq \infty$, and $I$ bounded or unbounded. Then there exists a function $\tilde{u}$ in $C(\overline{I})$ such that:

$$u = \tilde{u} \quad \text{a.e. in } I,$$

and

$$\tilde{u}(x) - \tilde{u}(y) = \int_x^y u'(t)dt \quad \forall x, y \in \overline{I}.$$
Appendix B

Principal Fiber Bundles

Either therefore the reality which underlies space must form a discrete manifoldness, or we must seek the ground of its metric relations outside it, in binding forces which act upon it.

(B. Riemann)

In 1917 Tullio Levi Civita [61] introduced a new fundamental concept in differential geometry, or as it was known at that time Calcolo Differenziale Assoluto, that is: parallel transport.

The question posed was about the meaning of “parallelism” on a surface, and in general on a manifold. Frankly, Levi Civita was concerned about reducing the formal apparatus which is necessary to introduce Riemannian curvature and to have a coherent covariant formulation. In [61] Levi-Civita states that Riemann, in his master thesis [62], had given some hints on how to characterize intrinsically the curvature, but had not precisely solved the problem. He stresses the fact that no mention on direzioni parallele in una varietà qualunque had ever been done before in order to study curvature intrinsically.

Stated in modern terms, there does not exist a canonical isomorphism between different tangent spaces on a differential manifold, so that in order to compare vectors in different tangent spaces one needs an extra structure, known as connection. The union of all the tangent spaces on a manifold is a very special case of a more general mathematical structure known as fiber bundle. As already stressed

\[1\] translated from the original work of Riemann [59] by W.K. Clifford in [60]
The development of fiber bundle theories in mathematics, on the one hand, and the one of gauge theories in physics, on the other, had proceeded independently for a very long time. But although mathematicians and physicists had been (apparently) studying different ideas, as a matter of fact they were investigating the same structures.

Roughly speaking a fiber bundle is a manifold which (locally) looks like a Cartesian product space. As a very special case, the tangent bundle to a manifold is a fiber bundle, whose base manifold is the manifold itself and whose fibers are the tangent spaces “attached” to every point on the manifold. For more precise definitions \[63\] and \[64\] represent classical references. In the present appendix we would like to introduce some ideas of the theory of connections on a principal fiber bundle, that is a bundle whose typical fiber inherits a Lie group structure. The idea is always the same: give a rule, that is a meaning to the words “horizontal” and “vertical”, when there is no canonical sense for them.
Let \((P, M, G, \pi)\) be a principal fiber bundle with total space \(P\) over a base
manifold \(M\) with Lie group \(G\) acting on the right on \(P\) and projection \(\pi\). Let
\(q \in P, \ x = \pi(q) \in M, \ p \in \pi^{-1}(x)\). The right group action on \(P\) is given by:

\[
\Phi : G \times P \to P : (g, p) \mapsto \Phi(g, p) = \Phi_g(p) = p \cdot g^{-1}.
\]

Roughly speaking the action of the group moves points in the bundle along the
fibers.

At any point \(q\) the tangent space to the bundle \(T_qP\) can be decomposed in two
spaces, one “parallel” to the fiber, the so-called **vertical subspace**, and one trans-
verse to the fiber, the **horizontal space**, so that \(T_qP = V_qP \oplus H_qP\) \(\text{[Figure B.1]}\).

On the one hand the vertical space can be uniquely determined by the condition:

\[
V_qP = \ker(\pi_\ast),
\]

but there is no canonical way of choosing the complementary space in \(T_qP\). But we
need it in order to define differentiation on the bundle. The assignment of such
horizontal spaces is called a **connection** in a bundle:

**Definition B.1.** A connection in a principal fiber bundle is a smoothly-varying
assignment to each point \(q \in P\) of a subspace \(H_qP\) of \(T_qP\) such that:

- \(T_qP = V_qP \oplus H_qP\quad \forall q \in P\),
- \((\Phi_g)_\ast(H_qP) = H_{\Phi_g(q)}P\quad \forall g \in G, \ q \in P\).

The first condition states that the horizontal space must be transverse to the fiber;
the second one, instead, says that if we take the horizontal space in \(q\) and push it
along the fiber using the action defined in \(\text{[B.1]}\) then the result is the same as if
we first push the point along the fiber and then form the horizontal subspace at
that point.

The bundle group is a Lie group and there is a natural identification of the tangent
space to a fibre with the Lie algebra \(\mathfrak{g}\) associated to the group. Then one can define
a connection in terms of a \(\mathfrak{g}\)-valued 1-form, since a choice of a horizontal subspace
defines a way of projection of \(T_qP\) onto \(T_qG\).
Thus we have a linear map $\omega : TP \to \mathfrak{g}$, that is a $\mathfrak{g}$-valued 1-form on $P$, the so-called connection 1-form. We are not going to delve into this equivalent definition and refer to the reference cited above.

We move on to the definition of parallel transport. Suppose we take a path in the bundle given by: $t \in [a, b] \subset \mathbb{R} \to q(t) \in P$ and we give the following definition:

**Definition B.2.** A path $q(t)$ is horizontal with respect to a given connection if the tangent vector $\dot{q}(t)$ lies in the horizontal subspace determined by the connection, $H_{q(t)}P$, $\forall t \in [a, b]$.

**Definition B.3.** Any path in the bundle $P$ which projects under $\pi$ on the same path in $M$ as does $q(t)$ is called a lift of $q(t)$.

Since horizontal subspaces are by definition in the kernel of the associated connection 1-form $\omega$, so that equivalently, $q(t)$ is horizontal w.r.t. the given connection if $\omega(\dot{q}(t)) = 0$, $\forall t$. Moreover, from the above definition it follows that if a lift of $q(t)$ is horizontal w.r.t. $\omega$, then it is called a horizontal lift. Then, for a horizontal lift the projection of the tangent vector $\dot{q}(t)$ onto the vertical space at $q(t)$ is zero, for every point on the manifold.

The interesting thing is that the horizontal lift of a closed curve is not in general closed and this is linked to the curvature of the manifold. Moreover, taken a horizontal lift for a closed path then, parallel transport can be interpreted in terms of an automorphism on $T_xM$, where $x = \pi(p)$ is a base point on the manifold. The set of the automorphisms obtained is named the holonomy group of $M$ in $x$, and it is an invariant object associated to the connection.

To be more concrete, let us call $T_\gamma$ the automorphism on $T_xM$ induced by the connection. Since after a turn around we have made our way back to the original fiber we have that a parallel transport uniquely determines an element $\alpha(\tilde{\gamma})$ on the fiber in $x$, where $\tilde{\gamma}$ is the horizontal lift of $\gamma$, such that:

$$T_\gamma(p) =: p \cdot \alpha(\tilde{\gamma}). \tag{B.3}$$

In equation (B.3) we are using the right action on the fiber. The element of the group $G$, $\alpha(\tilde{\gamma})$ is known as the holonomy of a curve $\tilde{\gamma}$ with respect to the given connection (Figure(B.2)). Clearly, since horizontal lifts of closed paths are, in general, not closed we have that $\tilde{\gamma}$ is closed if and only if: $\alpha(\tilde{\gamma}) = e$. 
Figure B.2: Starting from the path $\gamma$, we consider its horizontal lift with respect to a given connection; $\tilde{\gamma}$ in general is not closed. Then the holonomy associated is $\alpha(\tilde{\gamma})$.

We thus build up the holonomy group of the connection given at the point $p$ considering different closed curves in $M$ starting in $x$ and taking their horizontal lifts, that is:

$$\text{Hol}(p) := \{ \alpha(\tilde{\gamma}) : \gamma \text{ closed } \gamma(0) = \gamma(1) = \pi(p), \tilde{\gamma}(0) = p \}.$$  \hspace{1cm} (B.4)

It is easy to prove that $\text{Hol}(p)$ is a subgroup of $G$ and that in the context of gauge theories one has that:

$$\alpha(\tilde{\gamma}) = \mathcal{P} \exp \left( \int_\gamma A \right),$$  \hspace{1cm} (B.5)

where $\mathcal{P}$ stands for “path ordered” and $A$ is the connection 1-form. In the derivation of the Berry’s phase the anholonomy corresponded exactly to the term in the previous equation, which we had named $\gamma_n(C)$, where $C$ was the chosen closed path.
Appendix C

Schrödinger Operators on Intervals and the Wronskian

In this appendix we consider self-adjoint extensions of the Laplacian on finite intervals. In this particular case the boundary form will be linked to the Wronskian, showing a connection between ordinary differential equations and boundary forms.

Let $a, b \in \tilde{\mathbb{R}}$, where $\tilde{\mathbb{R}}$ is $\mathbb{R} \cup \{\pm \infty\}$, and $\Delta$ be the Laplacian operator defined over $C_0^\infty(a, b)$, which is dense in $L^2(a, b)$, and let $V \in L^2_{\text{loc}}(a, b)$ a real potential. Consider:

$$H = -\Delta + V,$$  \hfill (C.1)

the Hamiltonian of a nonrelativistic particle of mass $m = 1/2$. From von Neumann’s theory we infer that $n_+ = n_-$, so that $H$ admits self-adjoint extensions. As we have already stated one can study self-adjoint extensions of a Hermitian operator by considering suitable restrictions of its adjoint where the boundary form vanishes. We are not going to delve into the theory of self-adjoint extensions of the above minimal operator, rather we are going to state the following proposition:

**Proposition C.1.** The boundary form of $H$ defined above is given by:

$$\Gamma(\psi, \phi) = W_b[\psi, \phi] - W_a[\psi, \phi], \quad \psi, \phi \in \text{D}(H^*) = \mathcal{H}^2[a, b],$$  \hfill (C.2)

where $W_x[\psi, \phi] = \overline{\psi(x)}\phi'(x) - \overline{\phi'(x)}\psi(x)$ is the Wronskian of $\psi$ and $\phi$ at $x \in [a, b]$, and $\mathcal{H}^2[a, b]$ is the second space of Sobolev.
Then, according to some conditions which could be satisfied by the end-points (regular, singular, etc) one can give some sufficient conditions about the nature of self-adjoint extensions of (C.1). For further details [39].
Bibliography


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But most importantly, he has taught me that research in theoretical physics can be painstakingly hard and that, no matter how tired or frustrated you might be, you need to get up, try again and not to give up, because the joy of having found an answer to a question you had made, sweeps away all those nightmarish moments when you had felt defeated.

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