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# Towards the multiple-well Schrödinger ground state on tori. From Simon's approach to weak KAM

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*I think I can safely say that nobody understands quantum mechanics... Do not keep saying to yourself, if you can possible avoid it, "But how can it be like that?" because you will get 'down the drain', into a blind alley from which nobody has escaped. Nobody knows how it can be like that.*

- Richard Feynman, 1964-

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# Introduction

Very often, in molecules and solids, a quantum particle finds itself in a potential that has two or more local minima, separated by a barrier. For example, each electron in a hydrogen ($H_2$) molecule is attracted to both nuclei, so its external potential is a *double well* with a barrier in the middle. In particular, a double-well potential provides us a starting point for understanding periodic potentials with more than two wells, that are called *multiple-wells*.

In literature, the problem of a double well has been studied in details over the years and it is well known that it represents a clear example of quantum mechanical *tunneling* through a barrier.
Tunneling effect is one of the most important phenomena that only quantum mechanics has revealed and was discovered after the study of radioactivity. It was first noticed in 1927 by Friedrich Hund during the computation of the ground state of a double-well potential.
Its first application is due to George Gamow, when in 1928 provided a mathematical explanation for alpha decay. He was able to solve the Schrödinger equation for a nuclear potential and to derive a relationship between the lifetime of a particle and the energy of emission that is directly determined by the mathematical probability of tunneling. Later, Max Born understood the generality of tunneling and realized that it was not limited to nuclear physics, but was a general display of quantum mechanics concerning many different systems.
Today, a lot of phenomena related to tunneling are observed and applied in many areas of technology and microscopic science.
It is also important to underline that quantum and classical mechanics differ in the interpretation of this argument. In particular, classical mechanics states that particles, that do not have enough energy to overcome a barrier, will not be able to reach the other side. Instead, in quantum mechanics these particles, even though with a very small probability, can tunnel crossing the barrier.

The project of this thesis concerns the study in details of the articles of Barry Simon [32, 34], in which he analyzed the main properties of the Schrödinger operator

$$P(\hbar) = -\frac{\hbar^2}{2}\Delta + V(x)$$

for a double-well potential as shown in Fig. 1.

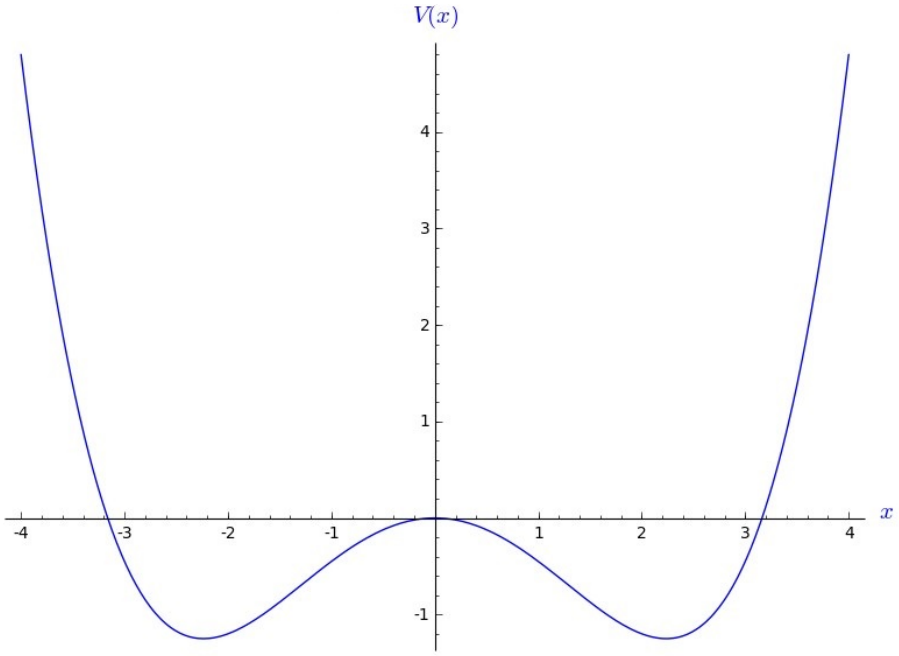


Figure 1: An example of double well potential.

We focus our attention on the leading asymptotics of the exponentially small splitting of the two lowest eigenvalues in the semi-classical limit $\hbar \to 0$. The second step is to examine more recent theories for finding a solid generalization of these results.
In this work, *semi-classical analysis* is the approach adopted in many questions. The purpose of this method is to recover, starting from the quantum mechanics, the classical mechanics [19], even though, sometimes, some important new non-classical facts are arising; in particular, the tunneling effect here studied.
After a detailed introduction to the elements both of mathematical analysis and of quantum mechanics useful to discuss fully the tunneling effect [11, 27, 34], we present the core of our work, that is the whole construction of the stationary solution of the Schrödinger equation on tori at the bottom of a multiple-well energy potential, generalizing the classical result by Simon for double wells. To do this, we use recent techniques completely different from those used by Simon –i.e., large deviation theory– such as viscosity solutions and weak KAM theory.

In some more details, the thesis is structured as following.
*Chapter 1* contains a short review of background knowledge about quantum mechanics, from the notion of Hilbert space to the three fundamental axioms [18, 31]. Here, we also present in details the WKB approximation [25], a method for finding approximate solutions discovered in 1926. Then, we introduce basic concepts regarding viscosity theory and we conclude the chapter with an exhaustive presentation of Simon main results [32, 34] about double

well problem and the objects that he used for the proofs.
In *Chapter 2* we focus on tunneling effect. We first analyze the general phenomenon, then we apply this theory to the cases of double and multiple wells. For this part we develop the original interpretation given by Helffer [19].
In *Chapter 3* we provide an elementary exposition of some basic concepts of weak KAM theory, that was introduced by Fathi, Mather and Aubry in order to study the dynamics of convex Hamiltonian systems. In particular we are interested in its link with evolutive and stationary Hamilton-Jacobi equations.
Finally, in *Chapter 4* we describe a new view on the multiple-well problem. In the first part we compute stationary solutions of the Schrödinger equation for a mechanical Hamiltonian for three different energy intervals. In the second section, we give a new proof and a generalization of the results for the double wells found by Simon.

# Chapter 1

# Preliminaries and Statements

The purpose of this chapter is first of all to refresh the main concepts of quantum mechanics and then to present some basic notions about viscosity solutions and tunneling. So we briefly provide the principal definitions and theorems that will be needed throughout the thesis.
For more information the reader can see the following references: [18, 25] for quantum mechanics and [6, 7, 8] for viscosity solutions.

## 1.1 Quantum mechanics overview

After the black body radiation theory by Planck (1900), the core of quantum theory is born around 1926 with Schrödinger equation. Although it is strongly based to the classical mechanics -it involves precisely the same potential energies-, quantum mechanics concerns mainly the study of the dynamics of particles and atoms at its fundamental level, giving often drastically different descriptions. The state of a particle, such as its position or momentum, is described by a statistical distribution derived from its wave function, solution of the Schrödinger equation.

### 1.1.1 Mathematical notions: Hilbert spaces and operators

Quantum theory is a mathematical model of the physical world. For the case of closed systems we can characterize this model by stating three axioms that specify how to represent states, observables and measurements [31].

**Definition 1.** (Hilbert Space)
A Hilbert space $\mathcal{H}$ is a

(i) complete complex vector space, that is, for $\psi, \varphi \in \mathcal{H}$ and $a, b \in \mathbb{C}$, then

$$a\psi + b\varphi \in \mathcal{H};$$

(ii) with a positive-definite scalar product

$$\begin{aligned} \langle\cdot|\cdot\rangle : \mathcal{H} \times \mathcal{H} &\longrightarrow \mathbb{C} \\ (\psi, \varphi) &\longmapsto \langle\psi|\varphi\rangle \end{aligned}$$

such that for all $\psi, \varphi, \varphi_1, \varphi_2 \in \mathcal{H}$ and $a, b \in \mathbb{C}$

$$\begin{aligned} \langle\psi|\varphi\rangle &= \overline{\langle\varphi|\psi\rangle} \\ \langle\psi|\psi\rangle &\geq 0 \\ \langle\psi|\psi\rangle = 0 &\Leftrightarrow \psi = 0 \\ \langle\psi|a\varphi_1 + b\varphi_2\rangle &= a\langle\psi|\varphi_1\rangle + b\langle\psi|\varphi_2\rangle. \end{aligned}$$

The dual space $\mathcal{H}^*$ of a separable Hilbert space $\mathcal{H}$ is also a vector space with the same dimension as $\mathcal{H}$. This identification motivates the *"bra"* and *"ket"* notation derived from the word bracket and introduced by Dirac.
Bra-vectors are elements of $\mathcal{H}^*$ that are written as $\langle\psi|$. Ket-vectors are elements of $\mathcal{H}$ that are written as $|\psi\rangle$. In addition, there exists a bijection between the Hilbert space $\mathcal{H}$ and its dual space $\mathcal{H}^*$, so each vector $|\psi\rangle \in \mathcal{H}$ corresponds to a vector in $\mathcal{H}^*$, which is thus denoted as $\langle\psi|$.
The application of the bra $\langle\psi|$ on the ket $|\varphi\rangle$ as the argument of the linear map is finally the "bracket" $\langle\psi|\varphi\rangle \in \mathbb{C}$.

Moreover, the scalar product is linear in the second argument and anti-linear in the first argument. It also induces a *norm*:

$$\begin{aligned} ||\cdot|| : \mathcal{H} &\longrightarrow \mathbb{R} \\ \psi &\longmapsto \sqrt{\langle\psi|\psi\rangle}, \end{aligned}$$

that is well-defined and in which $\mathcal{H}$ is complete.

Let see an example.

**Example 1.** Let $d^3x$ denote the Lebesgue measure in $\mathbb{R}^3$. Then we consider

$$L^2\left(\mathbb{R}^3\right) := \left\{\psi : \mathbb{R}^3 \to \mathbb{C} \mid \int_{\mathbb{R}^3} |\psi(x)|^2 \, d^3x < \infty\right\}$$

with the usual scalar product

$$\langle\psi_1|\psi_2\rangle := \int_{\mathbb{R}^3} \overline{\psi_1(x)}\psi_2(x) \, d^3x.$$

This is an infinite-dimensional Hilbert space, which is used to describe position and momentum of a particle in a three-dimensional space [31].

**Definition 2.** (Orthogonal Vectors)
A vector $\psi \in \mathcal{H}$ is called *unit vector* if $||\psi|| = 1$.
Two vectors $\psi, \varphi \in \mathcal{H}$ are said orthogonal to each other if $\langle\psi|\varphi\rangle = 0$. The subspace of vectors orthogonal to $\psi$ is denoted by

$$\mathcal{H}_{\psi^\perp} := \{\varphi \in \mathcal{H} | \langle\psi|\varphi\rangle = 0\}.$$

**Definition 3.** (Ray)
For every unit vector $|\psi\rangle \in \mathcal{H}$, the set

$$S_\psi := \{\lambda|\psi\rangle, \lambda \in \mathbb{C}\}$$

is called a ray in $\mathcal{H}$ with $|\psi\rangle$ as a representative.

Every element of a ray $S_\psi$ describes the same physical situation and the constant $\lambda \in \mathbb{C}$ can be arbitrarily chosen. So, since every ray corresponds to a possible state, given two states $|\psi\rangle$,$|\varphi\rangle$, another state can be constructed as the linear *superposition* of the two: $a|\psi\rangle + b|\varphi\rangle$, with $a, b \in \mathbb{C}$.

**Axiom 1. States** *A state is a complete description of a physical system. In quantum mechanics, a state is a ray in a Hilbert space.*

**Definition 4.** (Operator)
A linear map $A : \mathcal{H} \longrightarrow \mathcal{H}$ is called an operator on the Hilbert space $\mathcal{H}$. The set of all operators on $\mathcal{H}$ is denoted by $L(\mathcal{H})$.
The operator $A^* : \mathcal{H} \longrightarrow \mathcal{H}$ that satisfies

$$\langle A^*\psi|\varphi\rangle = \langle\psi|A\varphi\rangle, \qquad \forall\, |\psi\rangle, |\varphi\rangle \in \mathcal{H}$$

is called the *adjoint operator* to $A$.
If $A^* = A$, then $A$ is called *self-adjoint*.

**Axiom 2. Observables** *An observable is a property of a physical system that in principle can be measured. In quantum mechanics, an observable is a self-adjoint operator.*

**Definition 5.** (Eigenvalues and Eigenvectors)
Let $A$ be an operator on a Hilbert space $\mathcal{H}$. A vector $|\psi\rangle \in \mathcal{H} \setminus \{0\}$ is called eigenvector of $A$ with eigenvalue $\lambda \in \mathbb{C}$ if

$$A|\psi\rangle = \lambda|\psi\rangle.$$

The linear subspace that is spanned by all eigenvectors for a given eigenvalue $\lambda$ of an operator $A$ is called eigenspace of $\lambda$. Moreover, the set

$$\sigma(A) := \left\{\lambda \in \mathbb{C} | (A - \lambda I)^{-1} \text{ does not exist}\right\}$$

is called the *spectrum* of the operator $A$.

A self-adjoint operator in a Hilbert space $\mathcal{H}$ has a spectral representation and its eigenstates form a complete orthonormal basis in $\mathcal{H}$. We can express a self-adjoint operator $A$ as

$$A = \sum_n a_n E_n,$$

where $a_n$ is an eigenvalue of $A$ and $E_n$ is the corresponding orthogonal projection into the space of eigenvectors with eigenvalue $a_n$.

**Axiom 3. Measurement** *A measurement is a process in which information about the state of a physical system is acquired by an observer. In quantum mechanics, the measurement of an observable $A$ prepares an eigenstate of $A$ and the output of such measurement is the value of the corresponding eigenvalue.*

For simplicity, from now on we will consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$.
As regards the dynamics of the quantum system, the time evolution of the wave function is governed by a particular wave equation, called the *Schrödinger equation*. It was found in 1926 by Erwin Schrödinger and represents one of the greatest achievements of physics.

Given a particle of mass $m = 1$ and a potential energy $V(x)$, the Schrödinger equation in the position eigenbasis reads:

$$i\hbar\frac{\partial\Psi}{\partial t}(t,x) = -\frac{\hbar^2}{2}\Delta\Psi(t,x) + V(x)\Psi(t,x), \tag{1.1}$$

where $\hbar = h/2\pi$ is the reduced Planck's constant, $t \in \mathbb{R}$ and $x \in \mathbb{R}^n$.
We call a $L^2$-solution $\Psi$ the *wave function* and the quantity

$$p(t,x) := \frac{|\Psi(t,x)|^2}{\int_{\mathbb{R}^n}|\Psi(t,x)|^2 dx}$$

represents the *probability density*. So the probability to find the particle in the measurable set $\Omega \subset \mathbb{R}^n$ at the time $t$ is $P(t) = \int_\Omega p(t,x)dx$ [3].

The Schrödinger equation plays a role strictly analogous to Newton second law: given suitable initial condition $\Psi(0,x)$, the Schrödinger equation determines the wave function $\Psi(t,x)$ for all future time, just as in classical mechanics, given $x(0)$ and $\dot{x}(0)$, Newton law determine the position $x(t)$ for all future time.

Finally, we observe that Planck's constant $\hbar$ plays a fundamental role in all quantum phenomena. Its relative value determines the "extent of quantization" of a given physical system [25]. The transition from quantum mechanics to classical mechanics can be formally described as a passage to the limit often troublesome $\hbar \to 0$: this matter is the so-called *semi-classical analysis*.
Indeed, the purpose of such analysis is to understand, from a mathematical point of view, the general correspondence principle, due to Bohr, which states that one should recover, as the Planck's constant $\hbar$ tends to zero, the classical mechanics from the quantum mechanics.
This approach will be follow in many questions in this work.

### 1.1.2 The WKB approximation

In this thesis project we will analyze at first the case of a symmetrical double-well potential. It can be considered one of the most important potentials in quantum mechanics, because the solution contains the notion of a state as a

linear superposition of "classical" states, a concept which has become very important in quantum information theory.
This consists of a potential with two minima separated by a barrier.
There exist several analytic forms for the double well potential: the most common are the square double well potential, the quadratic form and the quartic form, that are illustrated in figure 1.1. It is important to note that the most important properties of double wells do not depend on the exact shape of the potential [22].

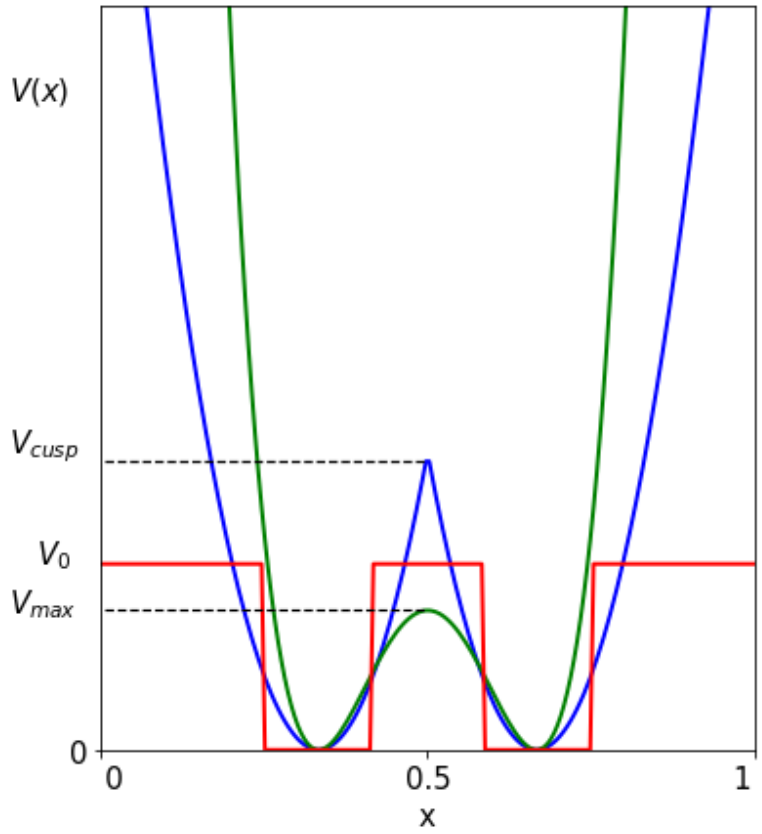


Figure 1.1: Three possible symmetrical double-well potentials are shown as a function of $x$. In red we have the square double well potential, that is piecewise constantly equal to $V_0$ and can be considered the most simple form. The quadratic form is shown in blue and it has a maximum (cusp) at the value $V_{\text{cusp}}$. Lastly, the quartic form is shown in green and it has a smooth maximum at the value $V_{\text{max}}$.

If the central barrier were *impenetrable*, we would simply have two detached harmonic oscillators and the energies would be doubly degenerate, since the particle could be in the left well or in the right one. When the barrier becomes *finite*, putting the two wells into "communication", the degeneracy is lifted and results a splitting of each of these levels into two neighbouring ones, corresponding to states in which the particle moves simultaneously in both wells [18].

The primary focus is often the calculation of the ground state splitting, but obviously many other levels can be obtained.
In literature, the treatment of this problem vary from qualitative discussion, as in [18, 25], to the calculation of an analytical solution, as in [28].
More often, the Wentzel-Kramers-Brillouin (WKB) approximation is used to find a solution. An important observation is that the WKB solution, when done fully, is very accurate, but on the other hand this method is only valid for certain potentials and requires considerably more work than the computation of the exact solution, that is accessible with elementary mathematics.

Now we proceed to investigate more closely this approach.
The WKB approximation is a method for finding approximate solutions and it is typically used for semi-classical calculations in quantum mechanics. The name comes from Wentzel–Kramers–Brillouin, who all developed it in 1926.
Given a particle of mass $m = 1$ and a potential energy $V(x)$, we want to study the stationary Schrödinger equation

$$-\frac{\hbar^2}{2}\Delta\Psi(x) + V(x)\Psi(x) = E\Psi(x), \qquad x \in \mathbb{R} \tag{1.2}$$

when $\hbar$ tends to 0. In our analysis, we suppose that $V(x)$ is continuous and bounded, i.e. $V_{\min} \leq V(x) \leq V_{\max}$, and that also the given energy level $E$ is chosen between the limit values $V_{\min}$ and $V_{\max}$. We show an example of such potential in Figure 1.2.
To do this approximation, we propose in equation (1.2) the following candidate structure:

$$\Psi(x) = e^{\frac{i}{\hbar}\sigma(x)},$$

where $\sigma(x)$ is a solution of

$$-\frac{\hbar^2}{2}\left\{\frac{i}{\hbar}\sigma''(x) - \frac{1}{\hbar^2}[\sigma'(x)]^2\right\} = E - V(x). \tag{1.3}$$

We introduce the classical momentum of the particle

$$p(x) = \sqrt{2[E - V(x)]},$$

that is a real quantity if we are in a classically accessible region.
So equation (1.3) can be written as

$$[\sigma'(x)]^2 - i\hbar\sigma''(x) = [p(x)]^2. \tag{1.4}$$

If the potential $V(x)$ vanishes, then $p(x) \equiv p = \sqrt{2E}$ is constant and the solutions of equation (1.4) are $\sigma(x) = \pm px$. As expected for a free particle problem, we get plane waves as energy eigenfunctions.

The basic idea of this method is that if the potential $V(x)$ varies slowly over distances of the wavelength, then also the phase of the solution $\Psi(x)$ will vary

slowly and we can neglect the term containing the second derivative $\sigma''(x)$. This is exactly equivalent to the semi-classical limit $\hbar \to 0$.
So we obtain the *zero approximation*:

$$[\sigma_0'(x)]^2 = [p(x)]^2 \quad \Rightarrow \quad \sigma_0'(x) = \pm p(x),$$

that means

$$\sigma_0(x) = \pm \int p(x)dx. \tag{1.5}$$

The approximation made in equation (1.4) is legitimate only if the second term on the left-hand side is small compared with the first, i.e. we must have $[\sigma_0'(x)]^2 \gg |i\hbar\sigma_0''(x)|$ or

$$1 \gg \left|\frac{\hbar\sigma_0''(x)}{[\sigma_0'(x)]^2}\right| \approx \left|\frac{\hbar}{[p(x)]^2}\frac{dp(x)}{dx}\right| = \left|\frac{\hbar}{[p(x)]^3}\frac{dV(x)}{dx}\right|.$$

It is evident from this that the semi-classical approximation becomes inapplicable if the momentum of the particle is too small or, equivalently, if the wavelength is big. In particular, it is clearly inapplicable near *turning point*, that is near points where the particle, according to classical mechanics, would stop and begin to move in the opposite direction. These points are given by the equation $p(x) = 0$, that means $E = V(x)$. As $p \to 0$, the wavelength tends to infinity, and hence cannot possibly be supposed small [25].

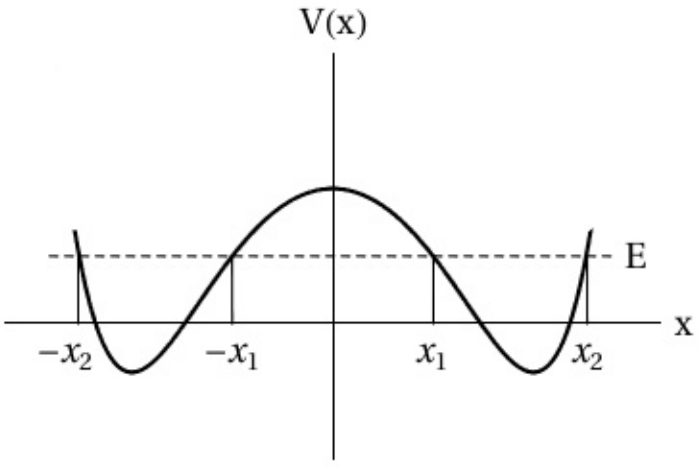


Figure 1.2: An example of continuous bounded potential. To apply the WKB approximation, the energy level $E$ should be chosen between $V_{\min}$ and $V_{\max}$. The points $\pm x_1$, $\pm x_2$, where $V(x) = E$, are the so-called turning points.

So $\sigma_0(x)$ is the exact solution for $\sigma(x)$ as $\hbar \to 0$.
Since the system is supposed almost classical in its properties, to find a better approximation we seek $\sigma(x)$ in the form of a series:

$$\sigma(x) = \sigma_0(x) + \frac{\hbar}{i}\sigma_1(x) + \left(\frac{\hbar}{i}\right)^2 \sigma_2(x) + ... \tag{1.6}$$

expanded in powers of $\hbar$.
Substituting this expression in equation (1.4), we obtain

$$\left[\sigma_0'(x) + \frac{\hbar}{i}\sigma_1'(x) + ...\right]^2 - i\hbar\left[\sigma_0''(x) + \frac{\hbar}{i}\sigma_1''(x) + ...\right] = [p(x)]^2$$

and equating the terms with the same power of $\hbar$, we get:

$$\begin{aligned} [\sigma_0'(x)]^2 &= [p(x)]^2 \\ 2\sigma_0'(x)\sigma_1'(x) + \sigma_0''(x) &= 0 \\ ... &= ... \end{aligned}$$

The first equation is exactly the (1.5), while from the second one we obtain

$$\begin{aligned} \sigma_1'(x) = -\frac{\sigma_0''(x)}{2\sigma_0'(x)} = -\frac{d}{dx}\frac{1}{2}\ln\sigma_0'(x) = -\frac{d}{dx}\ln\sqrt{|p(x)|} \\ \sigma_1(x) = \ln\frac{1}{\sqrt{|p(x)|}} + C. \end{aligned}$$

So at the first order of $\hbar$, the function $\sigma(x)$ is approximated by

$$\sigma(x) = \pm\int p(x)dx + \frac{\hbar}{i}\ln\frac{1}{\sqrt{|p(x)|}} + C \tag{1.7}$$

and the wave function $\Psi(x)$ by

$$\Psi(x) = C_1\frac{1}{\sqrt{|p(x)|}}\exp\left\{\frac{i}{\hbar}\int p(x)dx\right\} + C_2\frac{1}{\sqrt{|p(x)|}}\exp\left\{-\frac{i}{\hbar}\int p(x)dx\right\} \tag{1.8}$$

when $E > V(x)$.
The subsequent terms in the expansion (1.6) lead to the appearance, in the coefficients of the exponentials, of terms in the second and higher powers of $\hbar$ and it is not usually necessary to calculate them.

The presence of the factor $1/\sqrt{|p(x)|}$ in the wave function (1.8) has a simple interpretation. The probability of finding the particle at a point with coordinate between $x$ and $x + dx$ is given by the square $|\Psi|^2$, i.e. is essentially proportional to $1/p$. This is exactly what we should expect for a "semi-classical" particle, since in classical motion the time spent by a particle in the segment $dx$ is inversely proportional to the velocity.

In the *classically inaccessible* region, where $E < V(x)$, the function $p(x)$ is purely imaginary, so that the exponents become real. The wave function can be written in the form

$$\Psi(x) = C_1'\frac{1}{\sqrt{|p(x)|}}\exp\left\{-\frac{1}{\hbar}\int|p(x)|dx\right\} + C_2'\frac{1}{\sqrt{|p(x)|}}\exp\left\{\frac{1}{\hbar}\int|p(x)|dx\right\}.$$

In conclusion, we have built the WKB approximations of the wave function both in cases $E > V(x)$ and $E < V(x)$. But, as we have already said, this particular approximation cannot be used in correspondence of turning points, where $E = V(x)$ [25].

## 1.2 Viscosity solutions of Hamilton-Jacobi equations

In this section, we will study the notion of viscosity solution which was originally introduced by Crandall, Evans and Lions [6, 7, 8, 10] in 1983. We will consider a Lagrangian system on the n-dimensional torus $\mathbb{T}^n$ and the associated Hamilton-Jacobi equation.

Let us start by giving some general hypotheses [11].

**Definition 6.** (Tonelli Lagrangian)
A Lagrangian $L$ on the torus $\mathbb{T}^n$ is called a Tonelli Lagrangian if it satisfies the following properties:

(L1) $L : T\mathbb{T}^n \to \mathbb{R}$ is of class at least $C^2$;

(L2) $L$ is strictly convex in the fibers, i.e. the second partial derivative is positive definite as a quadratic form: $\frac{\partial^2 L}{\partial v^2}(x,v) > 0$ for all $(x,v)$;

(L3) $L$ is superlinear in each fiber, i.e.

$$\lim_{|v|\to+\infty} \frac{L(x,v)}{|v|} = +\infty.$$

In what follows, we will consider a Tonelli Lagrangian $L$ and the associated Hamiltonian $H$ via the Legendre transformation:

$$\begin{aligned} \mathbb{T}^n \times \mathbb{R}^n &\longrightarrow \mathbb{R} \\ (x,p) &\longmapsto H(x,p) = \sup_{v\in\mathbb{R}^n} \left(p\cdot v - L(x,v)\right), \end{aligned}$$

hence $p = \frac{\partial L}{\partial v}(x,v)$.
The Hamiltonian $H$ so defined is also Tonelli (in the variable $p$), in fact it verifies the following conditions:

(H1) $H(x,p)$ is continuous in both variables and of class $C^2$;

(H2) $H$ is convex in the second argument;

(H3) $\lim_{|p|\to+\infty} \frac{H(x,p)}{|p|} = +\infty$ uniformly in $x$.

**Remark.** The mechanical Lagrangian $L(x,v) = \frac{|v|^2}{2} - V(x)$ with $V$ the continuous potential and the associated Hamiltonian

$$H(x,p) = \frac{|p|^2}{2} + V(x)$$

are both Tonelli quantities.

### 1.2.1 Definition

We now provide the main definitions about this theory [11].

**Definition 7.** (Stationary H-J Equation)
The stationary Hamilton-Jacobi equation associated to the Hamiltonian $H$ is the equation

$$H(x, Du(x)) = c, \tag{1.9}$$

where $c$ is a constant.

**Definition 8.** (Evolutionary H-J Equation)
The evolutionary Hamilton-Jacobi associated to $H$ is the equation

$$\frac{\partial u}{\partial t}(t,x) + H\left(x, \frac{\partial u}{\partial x}(t,x)\right) = 0. \tag{1.10}$$

The latter form can be reduced to the stationary form $\tilde{H} = 0$ by introducing the Hamiltonian $\tilde{H}$ defined by

$$\tilde{H}(t, x, s, p) = s + H(x, p).$$

It is well known that it is usually impossible to find global $C^1$ solutions of equation (1.9). So it is necessary to admit more general weak classes of solutions.

**Definition 9.** (General Weak Solution)
We say that $u : \mathbb{T}^n \to \mathbb{R}$ is a general weak solution of (1.9), if it is Lipschitz and $H(x, Du(x)) = c$ almost everywhere.

Even though we admit solutions with possible singularities on a set of vanishing measure points, this definition is too general, because it provides many solutions and it would be useful if it gave a unique or a small number of solutions. We can verify this fact in the following example.

**Example 2.** Let $M = \mathbb{R}$ and we take $H(x, p) = p^2 - 1$. Then any continuous piecewise $C^1$ function $u$ with derivative equal to $\pm 1$ is a very weak solution of the stationary Hamilton-Jacobi equation

$$H(x, Du(x)) = 0.$$

In addition, there are even more of such solutions. In fact, if $A \subset \mathbb{R}$ is a measurable subset and $\chi_A$ its characteristic function, then the function

$$f_A(x) = \int_0^x 2\chi_A(t) - 1\, dt$$

is Lipschitz with derivative $\pm 1$ almost everywhere.

At the light of the above example, we need a sort of selection criteria and the appropriate sense of weak solution we will consider in this thesis project is the notion of *viscosity solution*.

The name "viscosity solution" is justified by the fact that the existence of solutions was obtained by the vanishing viscosity method:

$$\frac{\partial u_\varepsilon}{\partial t}(t,x) + H\left(x, \frac{\partial u_\varepsilon}{\partial x}(t,x)\right) = \varepsilon \Delta u_\varepsilon(t,x), \tag{1.11}$$

where $\varepsilon$ is a small parameter.
We want to understand if a solution $u_\varepsilon(t,x)$ of (1.11) for $\varepsilon \to 0$ tends to a function $u(t,x)$, solution (in some sense) of the limit equation (1.10).
This question is not so easy, because the regularizing effect of the right-hand term $\varepsilon \Delta u_\varepsilon(t,x)$ vanishes as $\varepsilon \to 0$ and we obtain an equation that has non regular solutions. The answer is that if

$$\lim_{\varepsilon \to 0} u_\varepsilon(t,x) = u(t,x) \tag{1.12}$$

uniformly, then $u(t,x)$ is a viscosity solution.
The problem is that the above definition is hardly to use, so Crandall, Evans and Lions found out an equivalent definition that requires subsolutions and supersolutions, overcoming partially the difficulties of the limit (1.12) [6].

**Definition 10.** (Viscosity Solution)
A function $u : (0,+\infty) \times M \to \mathbb{R}$ is a viscosity *subsolution* of equation (1.10) on the open subset $M \subset \mathbb{T}^n$, if for every $C^1$ function $\phi : (0,+\infty) \times M \to \mathbb{R}$ and every point $(t_0, x_0) \in (0,+\infty) \times M$ such that $u - \phi$ has a local maximum at $(t_0, x_0)$, we have (Fig. 1.3)

$$\frac{\partial \phi}{\partial t}(t_0,x_0) + H\left(x_0, \frac{\partial \phi}{\partial x}(t_0,x_0)\right) \leq 0.$$

A function $u : (0,+\infty) \times M \to \mathbb{R}$ is a viscosity *supersolution* of equation (1.10) on the open subset $M \subset \mathbb{T}^n$, if for every $C^1$ function $\psi : (0,+\infty) \times M \to \mathbb{R}$ and every point $(t_0, x_0) \in (0,+\infty) \times M$ such that $u - \psi$ has a local minimum at $(t_0, x_0)$, we have (Fig. 1.4)

$$\frac{\partial \psi}{\partial t}(t_0,x_0) + H\left(x_0, \frac{\partial \psi}{\partial x}(t_0,x_0)\right) \geq 0.$$

A function $u : (0,+\infty) \times M \to \mathbb{R}$ is said to be a viscosity *solution*, if it is both a subsolution and a supersolution.

Since we cannot restrict to differentiable functions, we use $\phi$ and $\psi$, called *test functions*, that are smooth and on which we can test the condition.
We can conclude that the equivalence between these two definitions made the viscosity theory a successful approach.

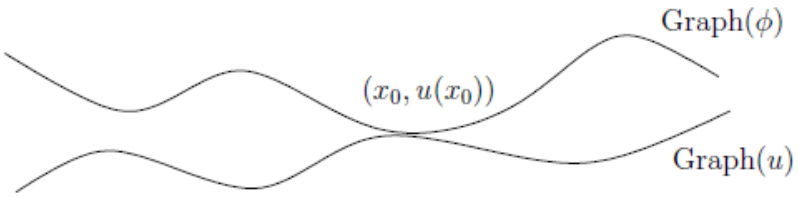


Figure 1.3: Subsolution in the stationary case: $\phi(x) \geq u(x)$, $u(x_0) = \phi(x_0)$ $\Rightarrow H(x_0, D\phi(x_0)) \leq c$.

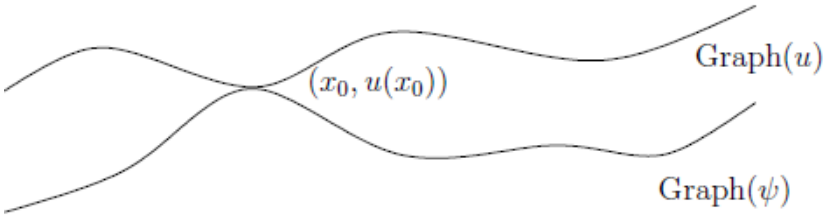


Figure 1.4: Supersolution in the stationary case: $\psi(x) \leq u(x)$, $u(x_0) = \psi(x_0)$ $\Rightarrow H(x_0, D\psi(x_0)) \geq c$.

We apply the viscosity conditions to the Example 2 given above.

**Example 3.** Let $M = \mathbb{R}$ and we take $H(x, p) = p^2 - 1$.
If we consider the stationary Hamilton-Jacobi equation $H(x, Du(x)) = 0$, we have that any Lipschitz function $u : \mathbb{R} \to \mathbb{R}$ with constant $\leq 1$ is a viscosity subsolution.
To verify this fact, we consider a $C^1$ function $\phi$ and $x_0 \in \mathbb{R}$ such that $\phi(x_0) = u(x_0)$ and $\phi(x) \geq u(x)$ for all $x \in \mathbb{R}$. We can write

$$\phi(x) - \phi(x_0) \geq u(x) - u(x_0) \geq -|x - x_0|.$$

For $x > x_0$, we have

$$\frac{\phi(x) - \phi(x_0)}{x - x_0} \geq -1$$

and passing to the limit $\phi'(x_0) \geq -1$. On the other hand, if $x < x_0$ we obtain that $\phi'(x_0) \leq 1$ and this yields $|\phi'(x_0)| \leq 1$. Therefore

$$H(x_0, \phi'(x_0)) = |\phi'(x_0)|^2 - 1 \leq 0.$$

So, we have shown that any very weak subsolution $u$, i.e. any Lipschitz function such that $H(x, Du(x)) \leq 0$ almost everywhere, is a viscosity subsolution.

In this example is essential the fact that the Hamiltonian $H$ taken into account is convex in the variable $p$.
We also observe that the two smooth functions $x \to x$ and $x \to -x$ are the only two classical solutions.
It is easy to check that the absolute value function $x \to |x|$, that is a subsolution and also a solution on $\mathbb{R} \setminus \{0\}$ is not a viscosity solution on the whole of $\mathbb{R}$. On the other hand, the function $x \to -|x|$ is a viscosity solution. It is smooth and a classical solution on $\mathbb{R} \setminus \{0\}$ and it is a subsolution everywhere.

### 1.2.2 Main results

We now analyze the main results about viscosity solutions that were enounced and proved by Anantharaman [2] and Gomes [17]. We recall that in our analysis we take $L$ a Tonelli Lagrangian, as we have specified in the introduction of this section.

Let start with a theorem due to Fathi that will be useful to us later [11].

**Theorem 1.** *The function $u : \mathbb{T}^n \to \mathbb{R}$ is a viscosity solution of equation (1.9) if and only if it solves the following fixed point problem:*
*for all $x \in \mathbb{T}^n$ and for all $t \geq 0$ ,*

$$u(x) = \inf_{\gamma} \left\{ u(\gamma(0)) + \int_0^t L(\gamma(s), \dot{\gamma}(s)) ds \right\} + ct \tag{1.13}$$

*where the inf is taken over all piecewise $C^1$ curves $\gamma : [0, t] \to \mathbb{T}^n$ such that $\gamma(t) = x$.*

We will see soon that all this does work just for a unique value $c \in \mathbb{R}$.
Now let prove that this new definition is a generalization of classical solutions.

**Theorem 2.** *A $C^1$ function $u : \mathbb{T}^n \to \mathbb{R}$ is a viscosity solution of the stationary Hamilton-Jacobi equation $H(x, Du(x)) = c$ on $\mathbb{T}^n$ if and only if it is a classical solution.*

*Proof.* We will prove the theorem shown the subsolution case. For the supersolution, the proof is analogous.
We suppose that the $C^1$ function $u$ is a viscosity subsolution. Because $u$ is $C^1$, we can use it as a test function. We have that $u - u = 0$, so every $x \in \mathbb{T}^n$ is a maximum, hence $H(x, Du(x)) \leq c$, $\forall x \in \mathbb{T}^n$.
Conversely, we suppose that $H(x, Du(x)) \leq c$ for each $x \in \mathbb{T}^n$.
But if $\phi : \mathbb{T}^n \to \mathbb{R}$ is $C^1$ and $u - \phi$ has a maximum at $x_0$, then the function $u - \phi$ must have derivative 0 at $x_0$. This means that $D\phi(x_0) = Du(x_0)$ and $H(x, D\phi(x_0)) = H(x, Du(x_0)) \leq c$. □

**Theorem 3.** *If $H$ is a Tonelli Hamiltonian, then viscosity solutions of equation (1.9) are Lipschitz and exist for a unique value of $c$.*

This special constant $c$ is called Mañé's critical value and we will properly define it in Chapter 3. However there might be, in general, several solutions.

Now we report the results found by Gomes [17] about the study of the stationary viscous Hamilton-Jacobi equation:

$$H(x, Du(x)) = c(\varepsilon) + \frac{\varepsilon}{2}\Delta u(x), \tag{1.14}$$

where the torus is equipped with a flat metric and $\Delta$ is the Laplacian. The parameter $\varepsilon$ is the viscosity coefficient.

**Remark.** Analysts usually work with equations in the form

$$H(x, Du(x)) = c(\varepsilon) - \frac{\varepsilon}{2}\Delta u(x), \tag{1.15}$$

but we prefer the form (1.14) because it seems more convenient for the approach we use. It is possible to pass from one form to the other by replacing $u$ with $-u$ and $H(x, p)$ with $H(x, -p)$.

With this notation, we can enunciate the following crucial theorem:

**Theorem 4.** *For any parameter $\varepsilon > 0$, there exists a unique real number $c(\varepsilon)$ for which the equation (1.14) has a periodic viscosity solution, that we denote $u_\varepsilon$. Moreover, the solution is $C^2$ and unique up to constants.*

**Remark.** When compared to the case $\varepsilon = 0$, this result is extremely interesting because, although $c(\varepsilon)$ is still unique, the viscosity solution of $H(x, Du(x)) = c$ is not unique up to constants. Thus, as Anantharaman and co. [2] did, the limit for $\varepsilon \to 0$ of such a solution has been called *physical solution*.

**Proposition 1.** *The quantity $c(\varepsilon)$ can be estimated independently of $\varepsilon$ by*

$$\inf_x H(x, 0) \leq c(\varepsilon) \leq \sup_x H(x, 0). \tag{1.16}$$

*Proof.* Suppose $u$ has a minimum at $x_0$. Then we have $-\frac{\varepsilon}{2}\Delta u(x_0) \leq 0$ and $Du(x_0) = 0$. Thus, from equation (1.14) we obtain

$$c(\varepsilon) = -\frac{\varepsilon}{2}\Delta u(x_0) + H(x_0, Du(x_0)) \leq H(x_0, 0) \leq \sup_x H(x, 0).$$

The other estimate is similar. □

**Example 4.** As example, we can consider the mechanical case, that is

$$H(x, p) = \frac{|p|^2}{2} + V(x)$$

with $x \in \mathbb{T}^n$ and $p \in \mathbb{R}^n$. We want to see the uniqueness of the related viscous Hamilton-Jacobi equation.
Let

$$\mathcal{H}\psi = \left(\frac{\hbar^2}{2}\Delta + V\right)\psi$$

the Schrödinger operator taken into account (note the unusual sign in front of the Laplacian) and the associated stationary equation results

$$\frac{\hbar^2}{2}\Delta\psi(x) + V(x)\psi(x) = c(\hbar)\psi(x). \tag{1.17}$$

We search for solutions in the form

$$\psi(x) = e^{-\frac{u(x)}{\hbar}}. \tag{1.18}$$

Thus, replacing this candidate structure in equation (1.17), we get:

$$\begin{aligned}
\frac{\hbar^2}{2}\nabla\left[-\frac{1}{\hbar}Du(x)e^{-\frac{u(x)}{\hbar}}\right] + V(x)e^{-\frac{u(x)}{\hbar}} &= c(\hbar)e^{-\frac{u(x)}{\hbar}} \\
\frac{1}{2}|Du(x)|^2e^{-\frac{u(x)}{\hbar}} - \frac{\hbar}{2}\Delta u(x)e^{-\frac{u(x)}{\hbar}} + V(x)e^{-\frac{u(x)}{\hbar}} &= c(\hbar)e^{-\frac{u(x)}{\hbar}} \\
\frac{1}{2}|Du(x)|^2 - \frac{\hbar}{2}\Delta u(x) + V(x) &= c(\hbar),
\end{aligned}$$

that is exactly the equation (1.14).
Following Theorem 4 with $\hbar$ fixed, we can conclude that there exists a unique number $c(\hbar)$ for which the equation

$$\frac{1}{2}|Du(x)|^2 + V(x) = c(\hbar) + \frac{\hbar}{2}\Delta u(x), \tag{1.19}$$

admits a periodic viscosity solution, that we denote $u_\hbar$.
Thus, we have that the stationary solution $\psi_\hbar(x) = e^{-\frac{u_\hbar(x)}{\hbar}}$ is an eigenfunction of the Schrödinger operator $\frac{\hbar^2}{2}\Delta + V(x)$ with eigenvalue $c(\hbar)$, i.e.

$$\mathcal{H}\psi_\hbar(x) = c(\hbar)\psi_\hbar(x).$$

Since the eigenfunction is positive, it has to be the ground state and the associated eigenvalue is simple [2].
We will see an analogous calculation in Chapter 4, where we will present the computation of the ground state of the Schrödinger equation on the torus.

## 1.3 Tunneling

It is well known that one of the sharp differences from classical mechanics concerns the ability of quantum particles to *tunnel* between two regions separated by a classically forbidden region.
Quantitative estimates of this phenomenon first appeared in work on lifetimes for *$\alpha$-decays*, but mathematical analysis of these ideas has always been made difficult by the fact that a precise definition of lifetime is not so easy. Alpha decay is a type of radioactive decay in which an atomic nucleus emits an alpha particle (helium nucleus) and thereby "decays" into a different atomic nucleus, with a mass number and an atomic number that are reduced.
Alpha particles were first described in the investigations of radioactivity by Ernest Rutherford in 1899 and in 1928 George Gamow solved the theory of alpha decay via tunneling. He discovered that this special particle is trapped in a potential well by the nucleus. Classically, it is forbidden to escape, but according to the principles of quantum mechanics, it has a tiny (but non-zero) probability of tunneling through the barrier and appearing on the other side to escape the nucleus. Gamow solved a model potential for the nucleus and derived a relationship between the half-life of the decay and the energy of the emission. For this reason this phenomenon is considered the first quantum tunneling process.
Later, Max Born understood that tunneling does not belong exclusively to nuclear physics, but also to other physical phenomena.
Another situation where tunneling is important, and which is in many ways clearer than lifetime calculations, concerns *multiple-well* problems.
We will move in this direction to explore more.
In particular, in the next section we summarize the theorems found by Simon [32, 34] in the case of *double wells*. He published his articles in 1983-1984 and viscosity theory was unknown yet.
In order to state our main achievement, generalizing the result by Simon to any number of wells, we need to introduce a metric discussed initially by Agmon [1] in his study of the decay of $L^2$ solutions of $(-\Delta + V)u = 0$ at infinity. It is very close to the metric used by Jacobi in his studies of classical mechanics. We have to underline that this metric has been crucial also in the Simon's framework.

### 1.3.1 Agmon metric

Let $V$ be a function on $\mathbb{R}^n$ such that:

(i) $V$ is $C^\infty$;

(ii) $V(x) \geq 0$ for all $x$ and $V$ is strictly positive at $\infty$, i.e. $\lim_{|x|\to\infty} V(x) > 0$;

(iii) $V$ vanishes at exactly two points $a, b$ and $\frac{\partial^2 V}{\partial x_i \partial x_j}(x)$ is a non-singular matrix for $x = a, b$.

**Definition 11.** Under the above hypotheses on $V$, we define the Agmon metric $\rho$ by

$$\rho(x,y) = \inf_{\gamma} \left\{ \int_0^1 \sqrt{2V(\gamma(s))}|\dot{\gamma}(s)|ds| \ \gamma(0) = x, \ \gamma(1) = y \right\}, \tag{1.20}$$

that is the geodesic distance in the Riemann metric $2V(x)|dx|^2$.

There exists an equivalent form of equation (1.20) found by Carmona-Simon [4]:

**Proposition 2.** *Let $\rho$ be given in (1.20). Then*

$$\rho(x,y) = \inf_{\gamma,T} \left\{ \frac{1}{2} \int_0^T |\dot{\gamma}(s)|^2 ds + \int_0^T V(\gamma(s))ds| \ \gamma(0) = x, \ \gamma(T) = y \right\}, \tag{1.21}$$

*where we minimize over $T$ also.*

*Proof.* Let $\tilde{\rho}$ denote the right-hand side of (1.21). To prove that $\rho = \tilde{\rho}$ we show the double inequality.
Since $ab \leq \frac{1}{2}(a^2 + b^2)$, we can consider $a = \sqrt{2V(\gamma(s))}$ and $b = |\dot{\gamma}(s)|$ and we obtain:

$$\sqrt{2V(\gamma(s))}|\dot{\gamma}(s)| \leq \frac{1}{2}\left(2V(\gamma(s)) + |\dot{\gamma}(s)|^2\right) = \frac{1}{2}|\dot{\gamma}(s)|^2 + V(\gamma(s)).$$

Using the fact that arc length is invariant under parametrization, we get that $\rho \leq \tilde{\rho}$.
Instead, to obtain the other inequality, given any path $\gamma$ for $\rho$, we reparametrize it so that $|\dot{\gamma}(s)| = \sqrt{2V(\gamma(s))}$ and use this new path as a trial function for $\tilde{\rho}$. So we have shown that $\tilde{\rho} \leq \rho$. □

**Remark.** At points where $V$ vanishes, one may not be able to reparametrize $\gamma$ if $T < \infty$ is required. Thus, we shift the path with a small change of arc length so that zeros of $V$ are avoided.
As a result of this fact, we note an important aspect: the minimum problem (1.20) always has a minimizing path.
If $x$ and $y$ are zeros of $V$, then (1.21) may not possess a minimizing path if $T < \infty$. If both endpoints are zeros, there exists a path parameterized by $(-\infty, \infty)$ so that

$$\lim_{T\to-\infty} \gamma(s) = x, \qquad \lim_{T\to\infty} \gamma(s) = y.$$

This minimizing path for equation (1.21) with $x = a$ and $y = b$ is called an *instanton* and it runs from $-\infty$ to $+\infty$.

We also observe that the quantity (1.21) is the classical mechanical action for a particle moving in a potential $-V$. We call it *Agmon Lagrangian*.

The application of Agmon estimates in semi-classical analysis appears along 1983 in three papers: one research announcement by B. Simon [32] showing for the first time the role of the Agmon definitions in the semi-classical context for the symmetric double-well problem, one article by Helffer-Sjöstrand [20] and a detailed version of his previous announcement by Simon [34] (the two last ones appeared in 1984).
For the special case of one dimension, there is a huge literature and Agmon estimates are not needed because one can work directly with WKB solutions and standard aspects of the theory of ordinary differential equations.

### 1.3.2 Double wells and large deviations: Simon theory

We are interested in studying the Schrödinger operator

$$P(\hbar) = -\frac{\hbar^2}{2}\Delta + V(x) \tag{1.22}$$

and finding the leading asymptotics of exponentially small splitting of the two lowest eigenvalues in the semi-classical limit $\hbar \to 0$.
We indicate with $E_0(\hbar), E_1(\hbar)$ the lowest eigenvalues with corresponding normalized eigenvectors $\Omega_0(\hbar), \Omega_1(\hbar)$.
We suppose the assumptions (i)-(iii) on $V$. In addition, we require that the ground state has a piece in both wells so that the second eigenvalue is exponentially close to the lowest, i.e. we assume that for all $\varepsilon$ small:

(iv)
$$\lim_{\hbar\to 0} \int_{|x-y|\leq\varepsilon} |\psi_0(\hbar, x)|^2 dx > 0, \qquad\qquad y = a, b.$$

This is a quite simple situation and, if we have a symmetry, hypothesis (iv) is thus automatic.

**Theorem 5.** *Let $P(\hbar)$ be given by (1.22) and $V$ obeys (i)-(iii). Then for each $n$, when $\hbar \to 0$, $P(\hbar)$ has at least $n+1$ eigenvalues, $E_0(\hbar), ..., E_n(\hbar), ...$ and*

$$\lim_{j\to\infty} \hbar E_j(\hbar) = e_j,$$

*where $e_0 \leq e_1 \leq e_2 \leq ...$ are the elements of the canonical basis.*

Intuitively, the meaning of this theorem is the following: when $\hbar \to 0$, the corresponding eigenvectors must live near $a$ or $b$, the two wells. Near $a$, the operator $P(\hbar)$ looks like a sum of harmonic oscillators, and similarly for $b$.

In the rest of this section, we discuss the ground state (lowest eigenvalue) where we will get upper and lower bounds on the difference and determine the exact asymptotics. The technique that has been used is path integral, specifically the method of large deviations.
The main result is the following [32, 34]:

**Theorem 6.** *Let $P(\hbar) = -\frac{\hbar^2}{2}\Delta + V(x)$ where $V$ is a function on $\mathbb{R}^n$ obeying $(i) - (iv)$. Then*

$$\lim_{\hbar\to 0} \{-\hbar \ln |E_1(\hbar) - E_0(\hbar)|\} = \rho(a, b), \tag{1.23}$$

*where $\rho(a, b)$ is the distance from $a$ to $b$ in the Agmon metric.*

This theorem is the first rigorous result on leading behaviour in multidimensional double wells and it says that tunneling is determined by the action of the instanton. It suggests that the asymptotics of $E_1 - E_0$ will be connected to exponential decay of eigenfunctions of $P(\hbar)$.

Theorem 6 is proven showing upper and lower bounds on $E_1 - E_0$ and we reduce the proof to results on the decay of the ground state of the Schrödinger operator $P(\hbar)$, i.e. to the normalized vector $\Omega_0(\hbar, x)$ satisfying

$$P(\hbar)\Omega_0(\hbar, x) = E_0(\hbar)\Omega_0(\hbar, x).$$

It is essential the following result [32, 34]:

**Theorem 7.** *If hypotheses (i)-(iv) hold, then for any $x$*

$$\lim_{\hbar\to 0} \{-\hbar \ln \Omega_0(\hbar, x)\} = \min\left(\rho(x, a), \rho(x, b)\right), \tag{1.24}$$

*where the limit is uniform on compact subset of $x$.*
*Moreover, for some $R$ and $d > 0$, if $|x| > R$*

$$|\Omega_0(\hbar, x)| \leq Ce^{-\frac{d|x|}{\hbar}}. \tag{1.25}$$

One can prove Theorem 7 by using the differential equation methods of Agmon. We prefer an alternative proof, requiring the method of large deviations, and we will use Brownian motion theory.
It is well known that Brownian motion controls the kernel of the semi-group $e^{-tH}$, so we need two important facts:

1. the operator $P = -\frac{1}{2}\Delta + V$ has a complete set of eigenfunction $\psi_n(x)$ and
$$e^{-tH}(x, y) = \sum_{n=1}^{\infty} e^{-tE_n}\psi_n(x)\psi_n(y);$$

2. the *formula of Feynman-Kac*, that relates the Schrödinger semi-group $e^{-tH}$ with generator $P$ to some integral over Brownian paths. In general, it establishes a link between parabolic partial differential equations (PDEs) and stochastic processes. It is extremely useful in order to have a qualitative picture of the solution, as well as to establish error estimates [16, 30].

Using this important formula and the method of large deviations, one obtains:

**Theorem 8.** *For each fixed $x, y, T$ we have that*

$$\lim_{\hbar \to 0} -\hbar \ln \left[ e^{-\hbar T P(\hbar)}(x, y) \right] = A(x, y; T), \tag{1.26}$$

*where the limit is uniform on compact sets of $x, y, T$ and where*

$$A(x, y; T) = \inf_{\gamma} \left\{ \int_0^T \frac{|\dot{\gamma}(s)|^2}{2} ds + \int_0^T V(\gamma(s)) ds | \, \gamma(0) = x, \, \gamma(T) = y \right\}. \tag{1.27}$$

Moreover, to get the upper bound in Theorem 7, we need

**Lemma 1.**

$$\lim_{T \to \infty} A(x, x; T) = \min(2\rho(x, a), 2\rho(x, b)) \tag{1.28}$$

*and the limit is uniform as $x$ runs through compact sets.*

*Proof.* When $T \to \infty$, the minimizing path for (1.27) must go to $a$ or $b$ for most of its time, to prevent the potential term in the action from diverging. For $T$ large, the minimizing path is a minimum action path from $x$ to $a$ (or $b$) run for time $\frac{T}{2}$ and then return to $x$. □

In the next chapters, we will discuss these important results at the light of the theory of viscosity solutions and other more recent contributions.

# Chapter 2

# Interaction between the wells

In this chapter, our intention is to give a self-contained presentation of the tunneling effect in a simple situation.
At first, we analyze the general phenomenon with its properties, then we apply this theory to the special cases of double wells and multiple wells.
This treatment partly follows the original interpretation given by Bernard Helffer in 1980 [19].

We work on the flat torus $\mathbb{T}^n$ equipped with the Agmon metric $Vdx^2$ and we go on with the study of the Schrödinger operator

$$P(\hbar) = -\frac{\hbar^2}{2}\Delta + V(x). \tag{2.1}$$

Our hypotheses are that the given energy level $E$ vanishes, i.e. $E = 0$ and let us take

$$\min V(x) \leq 0 < \lim_{|x|\to\infty} V(x).$$

We write down the following decomposition:

$$V^{-1}(]-\infty, 0]) = U_1 \cup U_2 \cup ... \cup U_N,$$

where the $U_j$ are called the *wells* and are disjoint, compact and such that $\delta(U_j) = 0$. The quantity $\delta$ represents the diameter associated to the Agmon metric, that is defined as $(V-E)_+dx^2$, where $dx^2$ is the Riemannian metric. This is exactly the Jacobi metric introduced in classical mechanics, but we have replaced $(E-V)$ by $(V-E)$ because we are interested in working in the classically forbidden domain $V \geq E$.
Associated to this metric, we define a natural distance $d(x, y)$, which is the infimum of the length of piecewise paths connecting the points $x$ and $y$.
Then, we indicate with $S_0$ the minimal distance between the different wells, that is

$$S_0 = \min_{i\neq j} d(U_i, U_j).$$

Now we proceed to define the following important problem:

**Definition 12.** (Dirichlet Realization)
Let $\mathcal{I}$ be a subset of $]0, h_0]$ admitting 0 as an accumulation point and suppose that there is a family of eigenfunctions $u_\hbar$ such that:

- $P_M(\hbar) \cdot u_\hbar(x) = (E + \lambda(\hbar))u_\hbar(x)$
- $||u_\hbar|| = 1$
- $\max(\lambda(\hbar), 0) \xrightarrow[\hbar \to 0]{} 0, \qquad \hbar \in \mathcal{I}.$

Then $P_M(\hbar)$ is called Dirichlet realization of the Schrödinger operator $P(\hbar)$ in $M$, where $M$ is a bounded regular open set containing $U = \{x \in \mathbb{T}^n : V(x) \leq E\}$.

Our purpose now is to associate to each well a Dirichlet problem in some open set $M_j$ containing $U_j$. We denote it $P_{M_j}(\hbar)$ and $\varphi_\alpha$ are the eigenfunctions of $P_{M_{j(\alpha)}}(\hbar)$, where $j(\alpha)$ is the first index for $\alpha = (j, k)$.

## 2.1 The tunneling effect

Let $\tilde{W}$ be the matrix that corresponds to the interaction between the different wells and we have that:

$$\tilde{W}_{\alpha,\beta} = \mathcal{O}\left(e^{-\frac{S_0}{\hbar}}\right) \qquad \text{for } j(\alpha) = j(\beta), \quad (2.2)$$

which means that each well does not present self-interaction terms.
We are interested in calculating $\tilde{W}_{\alpha,\beta}$ for $j(\alpha) \neq j(\beta)$ in a way which allow to study the effect of interaction.

**Remark.** If we have two wells $U_1, U_2$ and only one eigenvalue $\mu_1(\mu_2)$ attached to each well, then if

$$|\mu_1 - \mu_2| \geq e^{-\frac{\varepsilon_0}{\hbar}} \qquad \text{for some } 0 < \varepsilon_0 < S_0,$$

the tunneling effect does not change the basic properties and the two wells are independent, i.e. non resonant. In addition, $P(\hbar)$ admits two eigenvalues $\tilde{\mu}_1, \tilde{\mu}_2$ that are separate from each other by $e^{-\varepsilon_0/2\hbar}$ and the associated eigenfunctions are located in the neighborhood of $U_1$ and $U_2$. Thus, the problem of tunneling occurs in this situation that $\mu_1 - \mu_2$ is exponentially small for order $e^{-S_0/\hbar}$.

For this reason, we have to introduce two new hypotheses:

- $\mu_\alpha - \mu_\beta = \mathcal{O}(\hbar^\infty)$
- $\varphi_\alpha = \mathcal{O}(\hbar^{-N_0} e^{-d(x, U_{j(\alpha)})/\hbar}), \qquad N_0 \in \mathbb{N}.$

The first one is almost always verified if there is a symmetry between different wells which implies $\mu_\alpha = \mu_\beta$.

Now we present the following theorem:

**Theorem 9.** *Let $F$ be a closed subspace in a Hilbert space $\mathcal{H}$.*
*Under the above two hypotheses, the matrix $\mathcal{M}$ of the operator $P_{|F}(\hbar)$ in the orthonormal basis $(e_\alpha)$ is given by*

$$\mathcal{M} = diag(\mu_\alpha) + \tilde{W}_{\alpha,\beta} + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}}, \tag{2.3}$$

*with*

$$\begin{cases} \tilde{W}_{\alpha,\beta} = 0 & \text{if } d(U_{j(\alpha)}, U_{j(\beta)}) > S_0 \text{ or } j(\alpha) = j(\beta) \\ \tilde{W}_{\alpha,\beta} = \hbar^2 \int_\Gamma \left(\varphi_\alpha \cdot \frac{\partial \varphi_\beta}{\partial n} - \varphi_\beta \cdot \frac{\partial \varphi_\alpha}{\partial n}\right) dS_\Gamma & \text{if } d(U_{j(\alpha)}, U_{j(\beta)}) = S_0 \end{cases}$$

*where $\frac{\partial}{\partial n}$ is the exterior normal derivative to $\Gamma$ and $dS_\Gamma$ is the induced measure on $\Gamma$.*

**Remark.** This theorem is unsatisfactory for the moment, because we do not know enough about the exact behaviour of the eigenfunction $\varphi_\alpha$. The good thing is that from the definition of the quantity $\tilde{W}_{\alpha,\beta}$ it is evident that is necessary to know $\varphi_\alpha$ only in a neighborhood of the integrable set $\Gamma$.

### 2.1.1 Double well problem

Let now apply the theory of the previous section to the case of two wells $U_1, U_2$. We denote the eigenvalues of the Dirichlet realization $P_{M_j}$ by $\mu_j$, with $j = 1, 2$. Then we have:

$$\begin{aligned} &S_0 = d(U_1, U_2), \\ &\beta := \tilde{W}_{1,2} = \tilde{W}_{2,1} = \mathcal{O}(\hbar^{-N_0})e^{-\frac{S_0}{\hbar}}. \end{aligned}$$

From Theorem 9, we obtain that the matrix of $P_{|F}(\hbar)$ is simply:

$$\mathcal{M} = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix} + \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix} + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}}. \tag{2.4}$$

Thus, from equation (2.4) we get that the operator $P(\hbar)$ has two eigenvalues $\lambda_1, \lambda_2$ such that:

$$\lambda_{1,2} = \frac{\mu_1 + \mu_2 \pm \sqrt{4\beta^2 + (\mu_1 - \mu_2)^2}}{2} + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}},$$

hence we have

$$|\lambda_2 - \lambda_1| = \sqrt{4\beta^2 + (\mu_1 - \mu_2)^2} + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}}. \tag{2.5}$$

This relation is significant if:

$$\sqrt{4\beta^2 + (\mu_1 - \mu_2)^2} > C\hbar^\nu e^{-\frac{S_0}{\hbar}}$$

for some $\nu \in \mathbb{R}$, $C > 0$.
In the first remark of the previous section, we have already analyzed the non resonant case $|\mu_1 - \mu_2| \geq C\hbar^\nu e^{-\frac{S_0}{\hbar}}$.

Let us regard in details what happens when there exists an isometry $g$ such that $g \cdot U_1 = U_2$ and $g^2 = e$. So using the symmetry properties, the matrix (2.4) become

$$\mathcal{M}_g = \mu I_2 + \begin{pmatrix} 0 & \tilde{\beta} \\ \tilde{\beta} & 0 \end{pmatrix}, \tag{2.6}$$

where we have set $\tilde{\beta} = \beta + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}}$.
In this special case, the eigenvalues are $\lambda_{1,2} = \mu \pm \tilde{\beta}$.
If $|\beta| \geq C\hbar^\nu e^{-\frac{S_0}{\hbar}}$, the splitting between $\lambda_1$ and $\lambda_2$ results

$$|\lambda_2 - \lambda_1| = 2\beta + \mathcal{O}(\hbar^\infty)e^{-\frac{S_0}{\hbar}} \geq C'\hbar^\nu e^{-\frac{S_0}{\hbar}} \tag{2.7}$$

More precisely, the normalized eigenvectors $u_1, u_2$ in the basis $(e_1, e_2)$ are given by

$$u_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \qquad u_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}.$$

In particular, we can observe that:

- $u_1 + u_2 = \begin{pmatrix} \sqrt{2} \\ 0 \end{pmatrix}$ is localized near $U_1$
- $u_1 - u_2 = \begin{pmatrix} 0 \\ \sqrt{2} \end{pmatrix}$ is localized near $U_2$

and the probability to be near $U_1$ for $u_1$ is equal to the probability to be near $U_2$ for $u_2$.

**Remark.** Starting from a symmetric situation like this, Simon studied a new phenomenon, called by him the *flea of the elephant* [35], that is a small perturbation outside the wells. The approach we have used in this section is particularly adapted to the deepening of this original problem.

## 2.2 Multiple-well problem at the bottom

As we have seen in the preceeding section, Theorem 9 reduces the study of interaction between the different wells to the computation of the matrix $\tilde{W}_{\alpha,\beta}$. But formula (2.3) is quite implicit, because we need to know the behaviour of $\varphi_\alpha$, the eigenfunctions of the Dirichlet realization $P_{M_j}$.
To solve this problem, in this section we will use the WKB construction realized at the bottom to give more explicit results. We have already described in detail this useful approximation in the first chapter.

For the study of this more complex problem, the following assumptions are necessary:

- $E = 0 = \min V(x)$;
- $V^{-1}(0) = \bigcup_{j=1}^{N} U_j$ (disjoint union);
- $U_j = \{x_j\}$ and $V''(x_j) > 0$, for $j = 1, .., N$

and we define

$$S_0 = \inf_{j \neq k} d(x_j, x_k).$$

Then let $\Omega_j$ be the set consisting of $x_j$ and the union of the interiors of all minimal geodesics from $x_j$ to some point in $\mathbb{T}^n$ of length strictly less than $S_0$. Here we consider only geodesics $\gamma : [0, a] \to \mathbb{T}^n$ such that:

- $\gamma(t) \in \mathbb{T}^n \setminus \{x_1, .., x_N\}$
- $\gamma(t) \xrightarrow[t\to 0]{} x_j$.

We have that $\Omega_j$ is an open set and $d_j(x) := d(x, U_j)$ is of class $C^\infty$ on $\Omega_j$. We now enounce the following proposition about the construction of a WKB solution. It is a generalization of a more simple theorem for the case taken into account [19].

**Proposition 3.** *Under the above hypotheses, we can find a formal series*

$$E^{(j)}(\hbar) \sim \sum_{i=1}^{\infty} E_i^{(j)} \hbar^i \tag{2.8}$$

*and a formal symbol defined in* $\Omega_j$

$$a^{(j)}(x, \hbar) \sim \sum_{i=0}^{\infty} a_i^{(j)}(x) \hbar^i, \tag{2.9}$$

*such that with* $\theta_j(x, \hbar) = \hbar^{-\frac{n}{4}} \cdot a^{(j)}(x, \hbar) e^{-\frac{d_j(x)}{\hbar}}$, *we have in* $\Omega_j$

$$\left(P(\hbar) - E^{(j)}(\hbar)\right) \theta_j(x, \hbar) = \mathcal{O}(\hbar^\infty) e^{-\frac{d_j(x)}{\hbar}}. \tag{2.10}$$

At this point, we take $\mathcal{I}(\hbar) = [0, C\hbar]$, where $C$ is such that for some $\zeta \in \mathbb{N}$ we have:

- for $j = 1, .., \zeta$, the Dirichlet problem $P_{M_j}(\hbar)$ has exactly one eigenvalue in the interval $\mathcal{I}(\hbar)$;
- for $j = \zeta + 1, .., N$, $P_{M_j}(\hbar)$ has no eigenvalues in $\mathcal{I}(\hbar)$.

This situation is always possible. For $j = \zeta + 1, .., N$ the $\{x_j\}$ are called *non resonant wells* and for $j = 1, .., \zeta$ are said *resonant wells*.

We just denote $\tilde{W}_{\alpha,\beta}$ by $\tilde{w}_{j,k}$ and we want to compute it for $j \neq k$ such that $S_0 = d(x_j, x_k)$ with $j, k \in [1, .., \zeta]$.
The idea is to replace in formula (2.3) the Dirichlet eigenfunction $\varphi_j$ of $P_{M_j}(\hbar)$ by the corresponding WKB solution $\theta_j$. To do this, we only had to compare $\varphi_j$ to $\theta_j$ in a neighborhood of the set $\Gamma_{j,k}$ which is inside $\Omega_j$.

Let $\tilde{\Gamma}_{j,k}$ be the set of minimal geodesics joining $\Gamma_{j,k}$ to $\{x_j\}$.

**Theorem 10.** *If $\varphi_j$ is the eigenfunction of $P_{M_j}(\hbar)$ with eigenvalue $\mu_j$ in the interval $\mathcal{I}(\hbar)$ and if $\tilde{\chi}_j$ is a $C^\infty$ function equal to 1 in a neighborhood of $\tilde{\Gamma}_{j,k}$, we have*

$$\tilde{w} \equiv \tilde{\chi}_j(\varphi_j - \theta_j) = \mathcal{O}(\hbar^\infty) e^{-\frac{d_j(x)}{\hbar}}. \tag{2.11}$$

We can proceed with the computation of the interaction term $\tilde{w}_{j,k}$.
Let start from the definition in Theorem 9:

$$\tilde{w}_{j,k} = \hbar^2 \int_{\Gamma_{j,k}} \left( \varphi_j \cdot \frac{\partial \varphi_k}{\partial n} - \varphi_k \cdot \frac{\partial \varphi_j}{\partial n} \right) dS_{\Gamma_{j,k}}.$$

Using Theorem 10, we obtain:

$$\tilde{w}_{j,k} = \hbar^2 \int_{\Gamma_{j,k}} \left( \theta_j \cdot \frac{\partial \theta_k}{\partial n} - \theta_k \cdot \frac{\partial \theta_j}{\partial n} \right) dS_{\Gamma_{j,k}}$$

and applying Proposition 3 we get finally:

$$\tilde{w}_{j,k} = -\hbar^{1-\frac{n}{2}} \int_{\Gamma_{j,k}} \left[ a^{(j)} a^{(k)} \left( \frac{\partial d_k}{\partial n}(x) - \frac{\partial d_j}{\partial n}(x) \right) + \hbar \left( a^{(j)} \frac{\partial a^{(k)}}{\partial n} - a^{(k)} \frac{\partial a^{(j)}}{\partial n} \right) \right] \times \\ \times e^{-\frac{d_j(x) + d_k(x)}{\hbar}} dS_{\Gamma_{j,k}}.$$

We observe that $\frac{\partial d_k}{\partial n}(x)$ and $-\frac{\partial d_j}{\partial n}(x)$ are different of 0 and not very different of $V(x)$. Thus, we have $a^{(j)} a^{(k)} \left( \frac{\partial d_k}{\partial n}(x) - \frac{\partial d_j}{\partial n}(x) \right) \geq C > 0$ on $\Gamma_{j,k}$.
So this last inequality holds:

$$C \int_{\Gamma_{j,k}} e^{-\frac{d_j(x) + d_k(x)}{\hbar}} dS_{\Gamma_{j,k}} \leq -\hbar^{\frac{n}{2}-1} \tilde{w}_{j,k} \leq \frac{1}{C} \int_{\Gamma_{j,k}} e^{-\frac{d_j(x) + d_k(x)}{\hbar}} dS_{\Gamma_{j,k}} \tag{2.12}$$

for $C > 0$ sufficiently small.

Now we are ready to state the main theorem of this section.

**Theorem 11.** *Let the interval $\mathcal{I}(\hbar)$ as defined above, then for $j,k \in 1,...,\zeta$ such that $S_0 = d(x_j,x_k)$, there exists a constant $C>0$ sufficiently small such that:*

$$C\hbar^{\frac{1}{2}} \leq -\tilde{w}_{j,k}e^{\frac{S_0}{\hbar}} \leq \frac{1}{C}\hbar^{1-\frac{n}{2}}. \tag{2.13}$$

*Proof.* We start with the first inequality. Let $x_i$ be a point in the interior of $\Gamma_{j,k}$ such that $d(x_j,x_i)+d(x_i,x_k)=S_0$ and note that on $\Gamma_{j,k}$

$$d_j(x)+d_k(x) \leq S_0 + Cd(x,x_i)^2.$$

Then, using formula (2.12), we get the thesis

$$\begin{aligned} Ce^{-\frac{S_0}{\hbar}}\hbar^{\frac{n-1}{2}} &\leq -\hbar^{\frac{n}{2}-1}\tilde{w}_{j,k} \\ C\hbar^{\frac{1}{2}} &\leq -\tilde{w}_{j,k}e^{\frac{S_0}{\hbar}}. \end{aligned}$$

For the second inequality, we observe that since $d_j(x)+d_k(x) \geq S_0$, then we have

$$-\hbar^{\frac{n}{2}-1}\tilde{w}_{j,k} \leq \frac{1}{C}e^{-\frac{S_0}{\hbar}}$$

and this concludes the proof. □

**Remark.** This theorem can be empty if there are no wells $\{x_j\},\{x_k\}$ with $j,k \in 1,...,\zeta$ such that $S_0 = d(x_j,x_k)$. More precise results for this special situation are given in [21].

**Remark.** The importance of Theorem 11 is due to the fact that it can be considered an improvement of Theorem 6 of Simon, which says only that

$$\lim_{\hbar\to 0}\left[\hbar\ln(-\tilde{w}_{j,k})\right] = -S_0. \tag{2.14}$$

As regards the notation, we have:

- $S_0 = \rho(a,b)$ is the geodesic distance in the Agmon metric;
- $-\tilde{w}_{j,k} = |E_1(\hbar) - E_0(\hbar)|$ is exactly the splitting of the two lowest eigenvalue.

So, it represents an important step forward in tunneling literature.

### 2.2.1 The case $N = 2$

Now we want to apply the general results found in the previous section to the most simple case of a double well.
Let us consider the continuous potential

$$V(x) = \frac{1}{4}(x^2-1)^2,$$

which is shown in Figure 2.1.

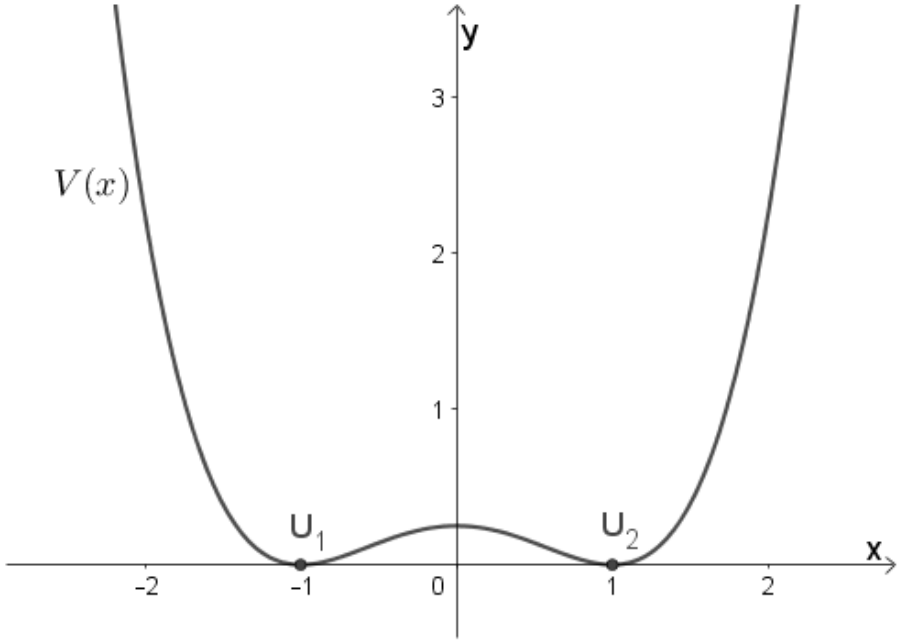


Figure 2.1: The potential $V(x)$ for the case taken into exam. This function is non-negative, symmetrical to the y-axis and vanishes in two points: $U_1$ and $U_2$.

Taking $E = 0$, we obtain two wells $U_1 = \{-1\}$, $U_2 = \{+1\}$ and we have $V^{-1}(0) = U_1 \cup U_2$.
We note also the even symmetry relation: $V(-x) = V(x)$.
Let us study in more detail the different steps of the general proof for this case.

Step 1: *The localized harmonic oscillator*
For the potential taken into consideration, we have that

$$V'(x) = (x^2 - 1)x, \qquad V''(x) = 3x^2 - 1.$$

In particular, $V''(-1) = V''(+1) = 2$ and the localized harmonic oscillator at the well $U_1$ is given by

$$-\hbar^2 \frac{d^2}{dy^2} + y^2, \tag{2.15}$$

where $y = x + 1$ is the new coordinate and $\hbar$ is the first eigenvalue. For the well $U_2$ we take $y = x - 1$. So we look for the spectrum in the interval $[0, 2\hbar]$.

Step 2: *The decay of eigenfunctions*
The Agmon distance in this case is given by

$$d(x, y) = \int_x^y |(t^2 - 1)| dt \tag{2.16}$$

with $x < y$.

The eigenfunctions $u_\hbar(x)$ of the Schrödinger operator $P(\hbar)$ associated to the eigenvalues have the following decay:

- Case $x < -1$ (and symmetrically $x > 1$):

$$u_\hbar(x) = \mathcal{O}(\hbar^{-N_0}) e^{-\frac{1}{\hbar}\int_x^{-1}\sqrt{V(t)}dt}$$

  uniformly for $x \in ]-M, -1]$, for each $M \in \mathbb{R}$.
- Case $-1 < x \leq 0$:

$$u_\hbar(x) = \mathcal{O}(\hbar^{-N_0}) e^{-\frac{1}{\hbar}\int_{-1}^{x}\sqrt{V(t)}dt}$$

  $\forall x \in ]-1, 0]$.
- Case $0 \leq x < 1$:

$$u_\hbar(x) = \mathcal{O}(\hbar^{-N_0}) e^{-\frac{1}{\hbar}\int_x^{1}\sqrt{V(t)}dt}$$

  $\forall x \in [0, +1[$.

Step 3: *The Dirichlet problems*
As we have seen in the general case, we define two Dirichlet problems: one in $M_1 = ]-M, 1-\eta[$ (see Fig. 2.2) and the other symmetrically in $M_2 = ]-1+\eta, M[$.
The constant $\eta > 0$ is chosen small and $M$ is such that

$$\int_{-M}^{1}\sqrt{V(t)}dt \geq 2S_0,$$

where the Agmon distance between the two wells results

$$S_0 = \int_{-1}^{+1}\sqrt{V(t)}dt = \frac{5}{6}.$$

We obtain that in $\mathcal{I}(\hbar)$ there exists only one eigenvalue $\mu_1(\hbar)$ of the Dirichlet problem $P_{M_1}(\hbar)$ and it admits an expansion of the form

$$\mu_1(\hbar) = \hbar + \sum_{j\geq 2} E_j \hbar^j.$$

By symmetry, the same is true for $P_{M_2}(\hbar)$ and we have

$$\mu_2(\hbar) = \mu_1(\hbar). \tag{2.17}$$

At that point, if we call $\varphi_1^{(\hbar)}(x)$ a normalized eigenfunction associated to $\mu_1(\hbar)$, it is evident that

$$\varphi_2^{(\hbar)}(x) := \varphi_1^{(\hbar)}(-x) \tag{2.18}$$

is a normalized eigenfunction for $P_{M_2}(\hbar)$, $\forall x \in M_2$.
In addition, we know that

$$\varphi_1^{(\hbar)}(x) = \mathcal{O}(\hbar^{-N_0}) e^{-\frac{1}{\hbar}\int_{-1}^{x}\sqrt{V(t)}dt} \tag{2.19}$$

uniformly for $x \in ]-M, 1-\eta[$.

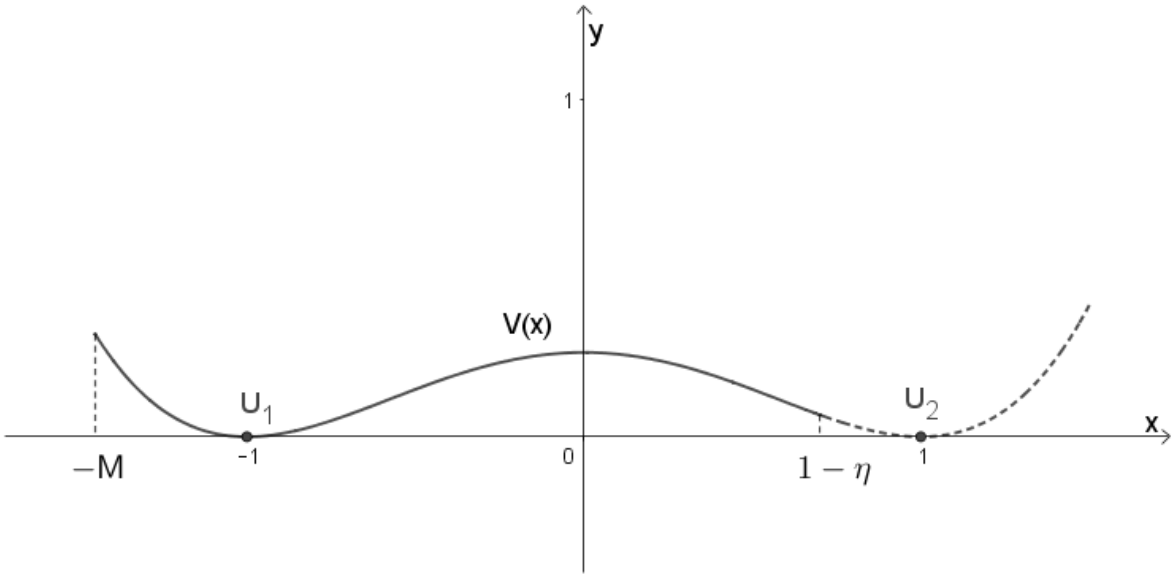


Figure 2.2: The potential $V(x)$ restricted to the set $M_1 = ]-M, 1-\eta[$. In this set is defined the Dirichlet problem $P_{M_1}(\hbar)$ with eigenvalue $\mu_1(\hbar)$.

Step 4: *The interaction matrix*
At first, let us define the basis that we will use for the calculation of the interaction matrix. We introduce

$$\Psi_1(\hbar)(x) = \chi_1(x)\varphi_1^{(\hbar)}(x), \tag{2.20}$$

where $\text{supp}\chi_1 \subset ]-M, 1-\eta[$.
By symmetry, we have that

$$\Psi_2(\hbar)(x) = \Psi_1(\hbar)(-x), \qquad x \in \mathbb{R}.$$

Then if $F$ is the spectral space of the operator $P(\hbar)$, we define

$$w_i = \Pi_F \Psi_i, \qquad i = 1, 2.$$

We observe that $(w_1, w_2)$ is a basis of $F$ and we have to orthonormalized it:

$$\vec{e} = \frac{1}{\sqrt{S}} \cdot \vec{w}$$

with $S = (w_i/w_j)$.

As we have studied at the beginning of the chapter, the matrix associated to $P_{|F}(\hbar)$ in the basis $\vec{e}$ is given by:

$$\mathcal{M} = \begin{pmatrix} \tilde{\mu} & \tilde{\beta} \\ \tilde{\beta} & \tilde{\mu} \end{pmatrix}, \tag{2.21}$$

where

$$\begin{cases} \tilde{\mu}(\hbar) = \mu_1(\hbar) + \mathcal{O}\left(e^{-\frac{2S_0}{\hbar}} \cdot e^{\frac{2\eta}{\hbar}}\right) \\ \tilde{\beta}(\hbar) = \beta(\hbar) + \mathcal{O}\left(\hbar^\infty\right) e^{-\frac{S_0}{\hbar}} \\ \beta(\hbar) = -\hbar^2 \left(\varphi_1^{(\hbar)}(0) \cdot \varphi'^{(\hbar)}_2(0) - \varphi'^{(\hbar)}_1(0) \cdot \varphi_2^{(\hbar)}(0)\right). \end{cases} \tag{2.22}$$

This simplified form is due to symmetry property.
Thus, from a direct calculation we obtain that the matrix $\mathcal{M}$ has two eigenvalues $\lambda_1(\hbar), \lambda_2(\hbar)$, with $\lambda_1 \leq \lambda_2$, such that

$$\lambda_{1,2}(\hbar) = \tilde{\mu} \pm \tilde{\beta}$$

(because we have supposed $\tilde{\beta} < 0$).
In conclusion, the splitting for this special case of a symmetrical double well is:

$$\begin{aligned} \lambda_2(\hbar) - \lambda_1(\hbar) &= -2\tilde{\beta}(\hbar) \\ &= 2\hbar^2 \left[\varphi_1^{(\hbar)}(0) \cdot \varphi'^{(\hbar)}_2(0) - \varphi'^{(\hbar)}_1(0) \cdot \varphi_2^{(\hbar)}(0)\right] + \mathcal{O}(\hbar^\infty) e^{-\frac{S_0}{\hbar}}. \end{aligned} \tag{2.23}$$

Step 5: *Computation of* $\varphi_1^{(\hbar)}(0)$ *and* $\varphi'^{(\hbar)}_1(0)$
The last thing we have to do is the calculation of the eigenfunction and its derivative for $x = 0$.
Let use the WKB approximation. From Theorem 10 and the definition of $\theta_j$ in Proposition 3, we know that $\varphi_1$ can be computed as

$$\varphi_1^{(\hbar)}(x) = \hbar^{-\frac{1}{4}} a(x, \hbar) e^{-\frac{1}{\hbar}\int_{-1}^{x} \sqrt{V(t)}dt}$$

for $x \in [-1, 1 - 2\eta[$, where

$$a(x, \hbar) \sim \sum_{j=0}^{\infty} a_j(x) \hbar^j.$$

Therefore, $a_0$ can be obtained by solving the transport equation:

$$a_0(x) = e^{-\int_{-1}^{x} \frac{(\sqrt{V})'(t) - 1}{2\sqrt{V(t)}} dt}. \tag{2.24}$$

From equations (2.23) and (2.24), we can conclude that the splitting results:

$$\lambda_2(\hbar) - \lambda_1(\hbar) = 4\hbar^{\frac{1}{2}} e^{-A} e^{-\frac{S_0}{\hbar}} + \mathcal{O}(\hbar^\infty) e^{-\frac{S_0}{\hbar}}, \tag{2.25}$$

where

$$A = \lim_{\varepsilon \to 0} \left[ \int_{-1+\varepsilon}^{1-\varepsilon} \frac{1}{2\sqrt{V(x)}} dx + \ln \varepsilon \right].$$

S. Coleman found the same formula in his work [5], but he gave a different heuristic proof using the method of instantons.
To conclude this discussion, we provide the following interpretation for the quantity $A$. Let

$$q(x,\xi) = \xi^2 - V(x)$$

the function that describes the motion in the forbidden region, where we have replaced $V$ by $-V$ as shown in Fig. 2.3.

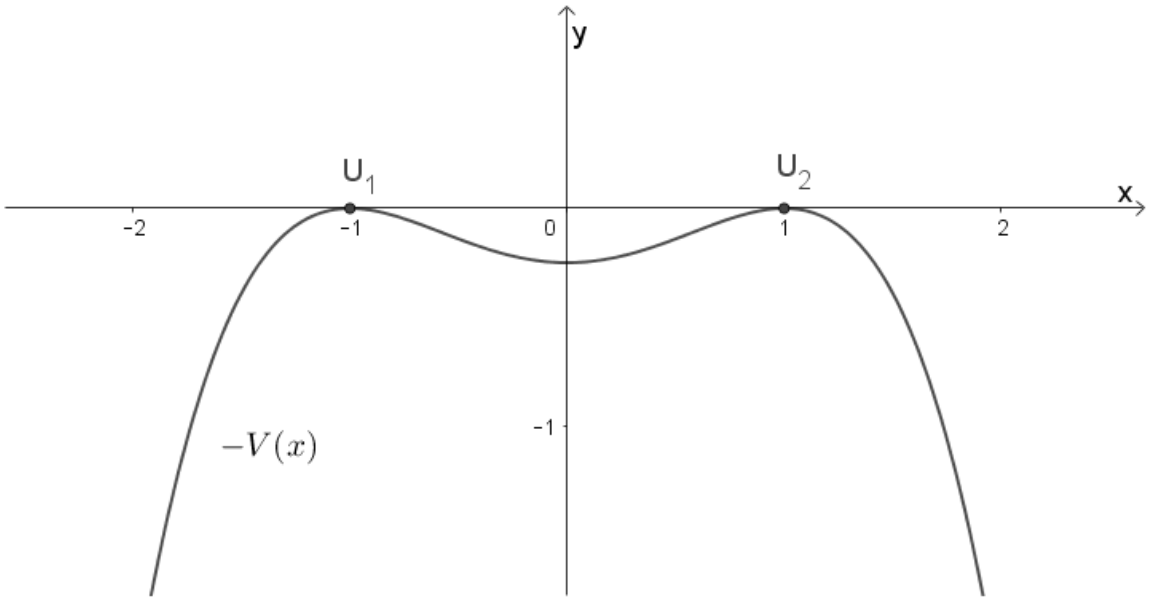


Figure 2.3: The potential $-V(x)$. We are interested in studying the motion between the two tops $U_1$ and $U_2$.

We would see what happens between the two maxima $U_1$ and $U_2$.
The motion equation results:

$$\frac{dx}{dt} = 2\xi = 2\sqrt{V(x)},$$
$$dt = \frac{1}{2\sqrt{V(x)}}dx.$$

Therefore,

$$T(\varepsilon) = \int_{-1+\varepsilon}^{1-\varepsilon} \frac{1}{2\sqrt{V(x)}}dx \tag{2.26}$$

is the time it takes to go from $(-1+\varepsilon)$ to $(1-\varepsilon)$.
In addition, we have that $T(\varepsilon) \underset{\varepsilon\to 0}{\longrightarrow} \infty$ like $-\ln\varepsilon \underset{\varepsilon\to 0}{\longrightarrow} \infty$ and so $A$ is called *principal part* of $T(\varepsilon)$.

# Chapter 3

# Weak KAM Theory

The origin of weak KAM theory and of his name is very intriguing. Classical KAM (from Kolmogorov-Arnol'd-Moser) theory began around 1950 by Kolmogorov [23, 24] and concerns perturbation theory of Hamiltonian integrable system: $H(q,p) = h(p) + \varepsilon f(q,p)$, $f \in \mathcal{O}(1)$.
Then, in 1988, among the specialists of the matter started to circolate the paper [26], where the authors (Lions, Papanicolaou and Varadhan) studied the so-called *cell problem*:
given a Tonelli Hamiltonian $H$, to determine, if possible:

(i) a function $\mathcal{S}(q,P) = q \cdot P + S(q,P)$;

(ii) a real function $K(P)$ such that

$$H\left(q, \frac{\partial \mathcal{S}}{\partial q}(q,P)\right) = K(P) \tag{3.1}$$

for all $q \in \mathbb{T}^n$, $P \in \mathbb{R}^n$.

Their result was that problem (3.1) is always solvable by a unique function $K(P)$ and for some Lipschitz solutions $S$ in the viscosity sense.
This led to the birth of a new weak theoretical framework [3].
From a strictly analytic mechanics point of view, we understand that if $\mathcal{S}(q,P)$ is smooth, we are concerning with an *integrable Hamiltonian system* and $\mathcal{S}$ is a generating function of a symplectomorphism reducing $H(x,p)$ to $K(P)$.

In this chapter we want to introduce some facts about weak KAM theory, that was developed by Fathi, Mather and Aubry in order to study the dynamics of convex Hamiltonian systems. The hypothesis of convexity is fundamental, in fact the richness of applications mainly comes from this remarkable convergence.
Another important fact from this new theory concerns the time asymptotic behaviour and it creates a bridge between evolutive and stationary Hamilton-Jacobi equations. The central reference on this argument is the still unpublished book of Albert Fathi [11].

## 3.1 The Mañé critical level

We start this section giving some general definitions about weak KAM theory. We denote by $M$ a compact and connected manifold. We also suppose that $M$ is provided with a Riemannian metric and $d$ is the distance on $M$ associated with this metric. Let $L$ be a Tonelli Lagrangian.

**Definition 13.** (Dominated Function)
Let $u : U \to \mathbb{R}$ be a function defined on $U \subset M$. If $c \in \mathbb{R}$, we say that $u$ is dominated by $L+c$ on $U$ if for each continuous piecewise $C^1$ curve $\gamma : [a, b] \to U$ we have

$$u(\gamma(b)) - u(\gamma(a)) \leq \int_a^b L(\gamma(s), \dot{\gamma}(s))ds + c(b - a).$$

We denote it by $u \prec L + c$.

We observe that the notion of dominated function does not use any differentiability assumption. Therefore, this definition is equivalent to the notion of viscosity subsolution given in Chapter 1.

**Definition 14.** (Calibrated Curve)
Let $u : U \to \mathbb{R}$ be a function and $c \in \mathbb{R}$ a constant, where $U \subset M$. We say that the piecewise $C^1$ curve $\gamma : [a, b] \to U$ is $(u, L, c)$-calibrated, if for every $t \leq t'$ we have

$$u(\gamma(t')) - u(\gamma(t)) \leq \int_t^{t'} L(\gamma(s), \dot{\gamma}(s))ds + c(t' - t).$$

Using these two definitions, we can give a useful characterization of $C^1$ solutions of the Hamilton-Jacobi equation, innovative because it does not require the derivative.

**Proposition 4.** *Let $L$ be a Tonelli Lagrangian defined on $M$. The $C^1$ function $u : U \to \mathbb{R}$ satisfies the Hamilton-Jacobi equation $H(x, Du(x)) = c$, $\forall x \in U$, if and only if it is dominated by $L + c$ and we can find a parameter $\varepsilon > 0$ and a curve $\gamma : [-\varepsilon, +\varepsilon] \to U$ that is $(u, L, c)$-calibrated and such that $\gamma(0) = x$ for every $x \in U$.*

We can proceed with the main definition of this part.

**Definition 15.** (Weak KAM Solution)
Under the above hypotheses, we define a weak KAM solution of negative type (resp. positive type) as a function $u : M \to \mathbb{R}$ for which there exists a constant $c \in \mathbb{R}$ such that

- u is dominated by $L + c$;
- we can define a $(u, L, c)$-calibrated $C^1$ curve $\gamma : ]-\infty, 0] \to M$ with $\gamma(0) = x$, $\forall x \in M$ (resp. $\gamma : [0, +\infty[ \to M$).

We denote the set of weak KAM solutions of negative and positive type by $\mathcal{S}_-$ and $\mathcal{S}_+$. In addition, we call $u_-$ an element of $\mathcal{S}_-$ and $u_+$ an element of $\mathcal{S}_+$.

**Definition 16.** (Conjugate Functions)
A pair of functions $(u_-, u_+)$ is said to be conjugate if $u_- \in \mathcal{S}_-$, $u_+ \in \mathcal{S}_+$ and $u_- = u_+$ on the Mather set $\mathcal{M}_0$.

From now on, we work in the flat torus $\mathbb{T}^n$ and our main goal is to define the *Mañé critical value*.
We suppose that the Hamiltonian $H : T^*\mathbb{T}^n \to \mathbb{R}$ is continuous, coercive and convex in the fibers.
In this context, if we consider the Cauchy problem for the evolutive Hamilton-Jacobi equation

$$\begin{cases} \frac{\partial S}{\partial t}(t,x) + H\left(x, \frac{\partial S}{\partial x}(t,x)\right) = 0 \\ S(0,x) = \sigma(x) \end{cases} \tag{3.2}$$

with $t \in (0,T)$, $x \in \mathbb{T}^n$, we know that it admits one and only one viscosity solution $S(t,x)$ which is continuous Lipschitz $C^{0,1}$.
This property cannot be extended to the stationary case

$$H(x, \nabla S(x)) = a, \qquad\qquad x \in \mathbb{T}^n. \tag{3.3}$$

But for a *unique* special value $a$, we can obtain also in this case a unique solution for equation (3.3). It is the so-called *Mañé critical value* and we denote it $c[0]$.
It is characterized by the fact that the corresponding Hamilton-Jacobi equation can be solved on the whole torus $\mathbb{T}^n$ in a viscosity sense. In other word, the quantity $c[0]$ indicates the unique energy level for which some global viscosity solution does exist.
For a rigorous definition, we have

$$\begin{aligned} c[0] &= \inf\{a \in \mathbb{R} : H(x, \nabla S(x)) = a \text{ has a subsolution}\} \\ &= \inf\{a \in \mathbb{R} : \exists u : \mathbb{T}^n \to \mathbb{R},\ u \prec L + a\}. \end{aligned}$$

The equivalence of these two definitions has been shown by Fathi [11] using the Lax-Oleinik semi-group, an object that we will introduce in the next section.

**Example 5.** If we take a mechanical Hamiltonian like

$$H(x,p) = \frac{|p|^2}{2} + V(x)$$

with $x \in \mathbb{T}^n$ and $p \in \mathbb{R}^n$, we obtain more simply that

$$c[0] = \max_{x \in \mathbb{T}^n} V(x). \tag{3.4}$$

This simplest form of $c[0]$ will be fundamental in the calculations of Chapter 4.

We can also give an elegant interpretation of the constant $c[0]$ using invariant measures with respect to Euler-Lagrange flow.

**Definition 17.** (Invariant Measure)
A probability measure $\mu$ on tangent bundle $T\mathbb{T}^n$ is said to be invariant with respect to Euler-Lagrange flow if

$$\int_{T(\mathbb{T}^n)} \Phi(\phi_t(x,v))d\mu = \int_{T(\mathbb{T}^n)} \Phi(x,v)d\mu$$

for each continuous and bounded function $\Phi$.

**Theorem 12.** *The Mañé critical value is given by*

$$c[0] = -\inf_{\mu}\left\{\int_{T(\mathbb{T}^n)} L(x,v)d\mu\right\}, \tag{3.5}$$

*where the lower bound is taken with respect to all Borel probability measures $\mu$ invariant by the Euler-Lagrange flow.*

The measures $\mu$ that realize the minimum are called *Mather measures.*

Now we want to explore more about asymptotic behaviour of the viscosity solutions for evolutive Hamilton-Jacobi equation.
In 2006 Davini and Siconolfi published a very general asymptotic theory [9] and they worked out results for coercive Hamiltonian functions. Among other things, they proved the following crucial theorem:

**Theorem 13.** *For any viscosity solution $S(t,x)$ of*

$$\frac{\partial S}{\partial t}(t,x) + H\left(x, \frac{\partial S}{\partial x}(t,x)\right) = 0, \qquad x \in \mathbb{T}^n, \tag{3.6}$$

*it holds that*

$$\lim_{t\to+\infty} ||S(t,\cdot) - (-c[0]t + \hat{S}(\cdot))||_{C^0} = 0, \tag{3.7}$$

*where $\hat{S}(x)$ is a global viscosity solution of the stationary Hamilton-Jacobi equation*

$$H(x, \nabla\hat{S}(x)) = c[0].$$

An interpretation of this theorem is that, asymptotically in the time, the viscosity solution $S(t,x)$ of equation (3.6) is uniformely blowing up as

$$S(t,x) \approx S_\infty(t,x) := -c[0]t + \hat{S}(x)$$

for $t$ large.

## 3.2 The Lax-Oleinik semi-group

We have seen that minimizers are fundamental in weak KAM theory, so we start this section with the definition of two new objects: the minimal action for a given time and the Peierls barrier. We will see that they satisfy some special properties.

**Definition 18.** (Minimal Action)
If $L$ is a Tonelli Lagrangian on the torus $\mathbb{T}^n$, for $t > 0$ fixed, we can define the function $h_t$ by:

$$\begin{aligned} \mathbb{T}^n \times \mathbb{T}^n &\longrightarrow \mathbb{R} \\ (x, y) &\longmapsto h_t(x, y) = \inf_{\gamma} \int_0^t L(\gamma(s), \dot{\gamma}(s)) ds, \end{aligned}$$

where the infimum is taken over all the continuous piecewise $C^1$ curves $\gamma : [0, t] \to \mathbb{T}^n$ with $\gamma(0) = x$ and $\gamma(t) = y$.
This quantity is called the minimal action to go from $x$ to $y$ in time $t$.

**Remark.** We observe immediately that for an "instanton" Lagrangian

$$L(x, v) = \frac{1}{2}|v|^2 + V(x)$$

the minimal action results

$$h_t(x, y) = \inf_{\gamma} \int_0^t \left[ \frac{1}{2}|\dot{\gamma}(s)|^2 + V(\gamma(s)) \right] ds$$

with $\gamma(0) = x$ and $\gamma(t) = y$. This quantity is exactly the propagator $A(x, y; t)$ defined in Chapter 1 in equation (1.27). This is the first rigorous connection found between the theory of Simon and the more recent weak KAM theory.

We proceed to sum up some important properties of this central object.

**Proposition 5.** *The minimal action $h_t$ satisfies:*

*(1) For each $x, y \in \mathbb{T}^n$, $t > 0$, we have*

$$h_t(x, y) \geq t \inf L.$$

*(2) For each $x, z \in \mathbb{T}^n$, $t, t' > 0$, we have*

$$h_{t+t'}(x, z) = \inf_{y \in \mathbb{T}^n} \{h_t(x, y) + h_{t'}(y, z)\}.$$

*(3) If $u : \mathbb{T}^n \to \mathbb{R}$ is a function, then $u \prec L + c$ if and only if $\forall\, x, y \in \mathbb{T}^n$, $\forall t > 0$, we have*

$$u(y) - u(x) \leq h_t(x, y) + ct.$$

*(4) For each $x, y \in \mathbb{T}^n$, $t > 0$ there exists an extremal curve $\gamma : [0, t] \to \mathbb{T}^n$ with $\gamma(0) = x$, $\gamma(t) = y$ and $h_t(x, y) = \int_0^t L(\gamma(s), \dot{\gamma}(s))$.*

Now we can keep on with the second definition of this section, due to Mather [27], which is strictly related to the first.

**Definition 19.** (Peierls Barrier)
We say that the Peierls barrier is a function $h : \mathbb{T}^n \times \mathbb{T}^n \to \mathbb{R}$ defined by

$$h(x,y) = \liminf_{t\to+\infty} \{h_t(x,y) + c[0]t\}.$$

Starting from the properties of the minimal action $h_t$, we obtain the next corollary.

**Corollary 1.** *The Peierls barrier $h$ satisfies the following properties:*

*(1) the values of the map $h$ are finite;*

*(2) the map $h$ is Lipschitzian;*

*(3) if $u \prec L + c[0]$, we have $h(x,y) \geq u(y) - u(x)$;*

*(4) $h(x,x) \geq 0$ for each $x \in \mathbb{T}^n$;*

*(5) $h(x,y) + h(y,z) \geq h(x,z)$;*

*(6) $h(x,y) + h(y,x) \geq 0$.*

Moreover, it is important also the following result, that relates the Peierls barrier with the weak KAM solutions.

**Theorem 14.** *For each $x, y \in \mathbb{T}^n$, we have the equality*

$$h(x,y) = \sup_{(u_-,u_+)} \{u_-(y) - u_+(x)\},$$

*where the sup is taken on pairs $(u_-, u_+)$ of conjugate functions.*

Now we are ready to introduce the main subject of this section: the *Lax-Oleinik semi-group*. In literature, it has been defined in different forms and it is well-known in PDE and in Calculus of Variations.
We call $C^0(\mathbb{T}^n, \mathbb{R})$ the set of continuous functions endowed with the topology of uniform convergence. Our main goal is to define a semi-group of non-linear operators $(T_t^-)_{t\geq 0}$ from $C^0(\mathbb{T}^n, \mathbb{R})$ into itself.

**Definition 20.** (Lax-Oleinik Semi-group)
The Lax-Oleinik semi-group is a family of non-linear operators

$$T_t^- : C^0(\mathbb{T}^n, \mathbb{R}) \longrightarrow C^0(\mathbb{T}^n, \mathbb{R})$$
$$u(\cdot) \longmapsto T_t^- u(x) := \inf_{\gamma} \left\{ u(\gamma(0)) + \int_0^t L(\gamma(s), \dot{\gamma}(s)) ds \right\},$$

where the infimum is taken over all absolutely continuous curves $\gamma : [0,t] \to \mathbb{T}^n$ such that $\gamma(t) = x$.

Using the definition of minimal action, we get

$$T_t^- u(x) = \inf_{y \in \mathbb{T}^n} \{u(y) + h_t(y, x)\}. \tag{3.8}$$

Now let us sum up some properties of the operators $T_t^-$.

**Proposition 6.** *Consider a function $u \in C^0(\mathbb{T}^n, \mathbb{R})$. Then, we have*

*(1) $T_{t+t'}^- = T_t^- \circ T_{t'}^-$ for each $t, t' \geq 0$ (Semi-group Property);*

*(2) $T_t^-(c + u) = c + T_t^- u$ for every constant $c \in \mathbb{R}$;*

*(3) if $u \leq v \Longrightarrow T_t^- u \leq T_t^- v$ for each $u, v \in C^0(\mathbb{T}^n, \mathbb{R})$ and $t > 0$ (Monotony);*

*(4) the maps $T_t^-$ are non-expansive for the norm $||\cdot||_\infty$, i.e. $\forall u, v \in C^0(\mathbb{T}^n, \mathbb{R})$, $\forall t \geq 0$,*

$$||T_t^- u - T_t^- v||_\infty \leq ||u - v||_\infty;$$

*(5) $T_t^-(\inf_{i \in I} u_i) = \inf_{i \in I} T_t^-(u_i)$, where $(u_i)_{i \in I}$ is a family of functions in $u$;*

*(6) if $c \in \mathbb{R}$ and $u$ is such that $u \prec L + c$, then the function $T_t^- u$ is finite valued and $T_t^- u \prec L + c$.*

A very interesting thing in our analysis is that the Lax-Oleinik operator solves the Cauchy problem for the evolutive Hamilton-Jacobi equation in the viscosity sense.

**Proposition 7.** *Let $H$ be an Hamiltonian associated to the Lagrangian $L$ via the Legendre transform. If we consider the Cauchy problem given in equation (3.2) with initial condition $\sigma(x)$, then we have that the function*

$$(t, x) \longrightarrow S(t, x) = T_t^- \sigma(x)$$

*is a viscosity solution for the problem on $(0, T) \times \mathbb{T}^n$.*

Notice that we did not make any convexity assumption. This is also called *Lax-Oleinik representation formula* for the viscosity solutions.
We continue with two important results concerning this semi-group.

**Proposition 8.** *The semi-group $T_t^-$ sends $C^0(\mathbb{T}^n, \mathbb{R})$ to itself and satisfies for all functions $u \in C^0(\mathbb{T}^n, \mathbb{R})$:*

- $\lim_{t \to 0} T_t^- u = u$;
- *the map $t \to T_t^- u$ is uniformly continuous.*

**Proposition 9.** *For each $t > 0$ there exists a constant $K_t$ such that, for every $u \in C^0(\mathbb{T}^n, \mathbb{R})$, the function $T_t^- u : \mathbb{T}^n \to \mathbb{R}$ is $K_t$-Lipschitzian.*

To conclude, we give the relationship between the semi-group $T_t^-$ and the weak KAM solutions of negative type.

**Proposition 10.** *Suppose that $u : \mathbb{T}^n \to \mathbb{R}$ is a function and $c \in \mathbb{R}$ a constant. We have the equality*

$$T_t^- u + ct = u$$

*for each $t \in [0, +\infty[$ if and only if $u$ is a negative weak KAM solution.*

## 3.3 Viscosity and Weak KAM

In this section we want to introduce the most important results about the quantities that we have just defined. In particular, we are interested in finding the connection between viscosity theory and the more recent weak KAM.

We start to prove the existence of negative weak KAM solution.

**Theorem 15.** *(Weak KAM Theorem)*
*There exists a function $u_- : \mathbb{T}^n \to \mathbb{R}$ which is a negative weak KAM solution with constant $c[0]$.*

So, this theorem yields an important fact: a weak KAM solution can only have the Mañé critical value as a constant.
Moreover, using Proposition 10 the weak KAM theorem can be reformulated as follows:

**Theorem 16.** *There exists a function $u_- : \mathbb{T}^n \to \mathbb{R}$ such that*

$$T_t^- u_- + c[0]t = u_- \tag{3.9}$$

*for each $t \in [0, +\infty[$.*

These equivalent theorems are very important in this context and there exist different proofs. We can now enounce the following theorem which yields immediately Theorem 15.

**Theorem 17.** *Let $L$ be a Tonelli Lagrangian and suppose that the function $u : \mathbb{T}^n \to \mathbb{R}$ is dominated by $L + c[0]$.*
*Then the quantity $T_t^- u + c[0]t$ converges uniformly to a continuous function $u_- : \mathbb{T}^n \to \mathbb{R}$ which is a negative weak KAM solution.*

In literature, one can find different statements of weak KAM theorem, for example in [12, 13] where is presented a version in the framework of Mather's theory.
The next theorem provide a useful characterization of $c[0]$ and is an immediate consequence of Theorem 15.

**Theorem 18.** *We have this characterization of the Mañé critical value:*

- *$c[0]$ is the only constant $c$ such that the semi-group $u \to T_t^- u + ct$ has a fixed point in $C^0(\mathbb{T}^n, \mathbb{R})$;*
- *$c[0]$ is the greatest lower bound of the set of the numbers $c \in \mathbb{R}$ for which there exists a function $u \in C^0(\mathbb{T}^n, \mathbb{R})$ with $u \prec L + c$.*

Our next step is to show the convergence of the Lax-Oleinik semi-group. This is a fundamental result and was studied by Fathi in his Comptes Rendus [11, 13, 14].

**Theorem 19.** *Let $L$ be a Tonelli Lagrangian and $T_t^-$ the Lax-Oleinik semigroup associated with $L$. Then for each $u \in C^0(\mathbb{T}^n, \mathbb{R})$ there exists the uniform limit of $T_t^- u + c[0]t$ for $t \to +\infty$.*

An important corollary of Theorem 19 is that the liminf in the definition of the Peierls barrier is indeed a limit.

**Corollary 2.** *For each $x, y \in \mathbb{T}^n$, we have*

$$h(x,y) = \lim_{t\to+\infty} h_t(x,y) + c[0]t.$$

*Moreover, the convergence is uniform.*

It is easy to see that this corollary is equivalent to Theorem 19, in fact for all $t > 0$, we have

$$T_t^- u(x) = \inf_{y\in\mathbb{T}^n} \{u(y) + h_t(y,x)\}, \tag{3.10}$$

as we have seen in the previous section.
In addition, there is another equivalent formulation for this theorem.

**Corollary 3.** *For each function $u \in C^0(\mathbb{T}^n, \mathbb{R})$ and $x \in \mathbb{T}^n$, we have*

$$\lim_{t\to+\infty} T_t^- u(x) + c[0]t = \inf_{y\in\mathbb{T}^n} \{u(y) + h(y,x)\}. \tag{3.11}$$

*Proof.* Using Equation (3.10) and Corollary 2, we obtain

$$\lim_{t\to+\infty} T_t^- u(x) + c[0]t = \lim_{t\to+\infty} \left\{ \inf_{y\in\mathbb{T}^n} [u(y) + h_t(y,x)] + c[0]t \right\} =$$
$$\lim_{t\to+\infty} \left\{ \inf_{y\in\mathbb{T}^n} [u(y) + h_t(y,x) + c[0]t] \right\} = \inf_{y\in\mathbb{T}^n} \left\{ \lim_{t\to+\infty} [u(y) + h_t(y,x) + c[0]t] \right\} =$$
$$\inf_{y\in\mathbb{T}^n} \left\{ u(y) + \lim_{t\to+\infty} [h_t(y,x) + c[0]t] \right\} = \inf_{y\in\mathbb{T}^n} \{u(y) + h(y,x)\}.$$

□

We finish this section showing the connection between weak KAM solutions and viscosity solutions. We will conclude that they are exactly the same.

**Theorem 20.** *Let $L$ be a Tonelli Lagrangian on the flat torus $\mathbb{T}^n$ and $H$ its associated Hamiltonian. A continuous function $u : U \to \mathbb{R}$ is a viscosity subsolution of the stationary Hamilton-Jacobi equation $H(x, Du(x)) = c$ on the open subset $U \subset \mathbb{T}^n$ if and only if $u \prec L + c$.*

The main theorem is the following:

**Theorem 21.** *Let $L$ be a Tonelli Lagrangian on the flat torus $\mathbb{T}^n$ and $H$ its associated Hamiltonian. A continuous function $u : \mathbb{T}^n \to \mathbb{R}$ is a viscosity solution of $H(x, Du(x)) = c$ if and only if it is Lipschitz and for each $t \geq 0$ satisfies the following relation*

$$u(x) = T_t^- u(x) + ct.$$

*Moreover, we have $c = c[0]$.*

# Chapter 4

# A new view on the multiple-well problem

In this chapter our purpose is to give a new proof and generalize the results for the double well problem found by Simon [32, 34].
He worked on this topic in the 1980s and his theory was very innovative for the time. As we have shown in Section 1.3.2, his achievements are mainly based on the method of large deviations and the Agmon metric.
We aim to build a solid generalization of these theorems for the case of a multiple-well problem using techniques completely different from those used by him. In particular, we will leverage more recent theories such as viscosity solutions and weak KAM, that we have deeply illustrated in the previous chapters.

In the first part of the chapter we compute stationary solutions of the Schrödinger equation for a mechanical Hamiltonian for three different energy intervals and we will find out that we have to use a specific approach for each case. Then in the second section we focus on the properties of the ground state and we will get to lay down the main achievement of this work.

## 4.1 Stationary solutions of Schrödinger equation on tori

In what follows we consider a mechanical Hamiltonian

$$\begin{aligned} H : \mathbb{T}^n \times \mathbb{R}^n &\longrightarrow \mathbb{R} \\ (x,p) &\longmapsto H(x,p) = \frac{|p|^2}{2} + V(x) \end{aligned}$$

and we take the potential energy to be continuous and bounded, such that $V_{\min} = 0 \leq V(x) \leq V_{\max}$.
We want to analyze the behaviour of stationary solutions of the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t}(t,x) = -\frac{\hbar^2}{2}\Delta\psi(t,x) + V(x)\psi(t,x), \tag{4.1}$$

where $x \in \mathbb{T}^n$ and $t \in \mathbb{R}$.
The associated operator is

$$\mathcal{H}\psi = \left(-\frac{\hbar^2}{2}\Delta + V\right)\psi.$$

We focus our attention on these *three* energy intervals: $(i)$ $E \geq V_{\max}$, $(ii)$ $0 < E < V_{\max}$ and $(iii)$ $E = 0 = V_{\min}$, that are different from a topological point of view.
We propose the following candidate solution:

$$\varphi(x) = e^{\frac{i}{\hbar}S(x)}, \tag{4.2}$$

where $S(x) = \rho(x) + i\sigma(x)$ with $\rho, \sigma \in \mathbb{R}$.

Let start our analysis.

*case (i)* : $E \geq V_{\max}$

If we search for a stationary solution, we have to consider

$$\psi(t,x) = \varphi(x)e^{-\frac{i}{\hbar}Et}. \tag{4.3}$$

Indeed, substituting this expression into equation (4.1), we obtain

$$\begin{aligned} i\hbar\left[\varphi(x)\left(-\frac{i}{\hbar}Ee^{-\frac{i}{\hbar}Et}\right)\right] &= -\frac{\hbar^2}{2}\nabla\cdot\left[\nabla\varphi(x)e^{-\frac{i}{\hbar}Et}\right] + V(x)\varphi(x)e^{-\frac{i}{\hbar}Et} \\ \varphi(x)Ee^{-\frac{i}{\hbar}Et} &= -\frac{\hbar^2}{2}\Delta\varphi(x)e^{-\frac{i}{\hbar}Et} + V(x)\varphi(x)e^{-\frac{i}{\hbar}Et} \\ -\frac{\hbar^2}{2}\Delta\varphi(x) + V(x)\varphi(x) &= E\varphi(x). \end{aligned}$$

This means that $\varphi(x)$ is exactly a solution of the stationary Schrödinger equation. Now, we put the form (4.2) into the last equation:

$$\begin{aligned} -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{i}{\hbar}\nabla S(x)e^{\frac{i}{\hbar}S(x)}\right) + V(x)e^{\frac{i}{\hbar}S(x)} &= Ee^{\frac{i}{\hbar}S(x)} \\ -\frac{i\hbar}{2}\Delta S(x) + \frac{|\nabla S(x)|^2}{2} + V(x) &= E. \end{aligned}$$

In a semi-classical context ($\hbar \to 0$), we can neglect the perturbation $-\frac{i\hbar}{2}\Delta S(x)$ and thus we meet the following stationary Hamilton-Jacobi equation:

$$\frac{|\nabla S(x)|^2}{2} + V(x) = E. \tag{4.4}$$

In section 1.2 about viscosity solutions we have established in Theorem 3 that the stationary Hamilton-Jacobi equation (1.9) admits a viscosity solution only for a unique value of $c$, that is exactly the Mañé critical value $c[0]$. We have defined this quantity and its properties in Chapter 3

and we have also seen that is a fundamental object in weak KAM theory. Therefore, in this specific situation $S(x)$ is a global solution for equation (4.4) and exists in the sense of viscosity if and only if $E = c[0]$. In the particular case of a mechanical Hamiltonian, we have remarked in Section 3.1 that $c[0] = V_{\max}$.
So, summing up, in this first case the semi-classical analysis provides that there exists a viscosity solution only for the lower bound $E = V_{\max}$.

*case (ii)* : $0 < E < V_{\max}$
In this case, the approach that we use is the WKB approximation. The exact procedure and the motivations of this method have been explained in details in Section 1.1.
We find out purely oscillating WKB solutions, i.e. we neglect $\mathcal{O}(\hbar)$ terms. When $E > V(x)$ the solution is an imaginary exponential, so it involves the real part $\rho(x)$. Instead, in the classically inaccessible region $E < V(x)$ the exponential becomes real, so the imaginary part $\sigma(x)$ of the function $S(x)$ is involved.
At the end of the calculations, a very accurate work is required to check continuity conditions between the different regions.

*case (iii)* : $E = 0 = V_{\min}$
This is the most interesting case in our analysis.
We want to see what happens at the minimum level $E = 0$. We have:

$$\begin{aligned}
0 &= -\frac{\hbar^2}{2}\Delta e^{\frac{i}{\hbar}S(x)} + e^{\frac{i}{\hbar}S(x)}V(x) \\
0 &= -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{i}{\hbar}\nabla S(x)e^{\frac{i}{\hbar}S(x)}\right) + e^{\frac{i}{\hbar}S(x)}V(x) \\
0 &= -\frac{i\hbar}{2}\Delta S(x)e^{\frac{i}{\hbar}S(x)} + \frac{|\nabla S(x)|^2}{2}e^{\frac{i}{\hbar}S(x)} + e^{\frac{i}{\hbar}S(x)}V(x) \\
0 &= -\frac{i\hbar}{2}\Delta S(x) + \frac{|\nabla S(x)|^2}{2} + V(x). \qquad (4.5)
\end{aligned}$$

We are looking for $S$ of the structure $S(x) = \rho(x) + i\sigma(x)$, so equation (4.5) can be written as

$$0 = -\frac{i\hbar}{2}\left[\Delta\rho(x) + i\Delta\sigma(x)\right] + \frac{1}{2}\left[|\nabla\rho(x)|^2 - |\nabla\sigma(x)|^2 + 2i\nabla\rho(x)\cdot\nabla\sigma(x)\right] + V(x). \qquad (4.6)$$

We separately analyze real and imaginary part of the last equation.

As regards the *imaginary part*, in the previous calculations we have obtained:

$$0 = -\frac{\hbar}{2}\Delta\rho(x) + \nabla\rho(x)\cdot\nabla\sigma(x). \qquad (4.7)$$

We want to prove that a viscosity solution of equation (4.7) can exist if and only if $\rho(x)$ is a constant quantity.

Indeed, in the semi-classical limit $\hbar \to 0$, we get:

$$\nabla\rho(x) \cdot \nabla\sigma(x) = 0$$

and, as a consequence, $\rho(x)$ has to be an integral of motion of the vector field

$$\dot{x} = X(x) = \nabla\sigma(x),$$

where $x \in \mathbb{T}^n$. A point $x^*$ that realizes the maximum is a point of asymptotically stable equilibrium, so every integral of motion has to be trivial, i.e. equal to a constant.
Since we are looking for semi-classical solutions, we take from now

$$\rho(x) \equiv 0.$$

Now we focus on the *real part*. From equation (4.6), we get:

$$0 = \frac{\hbar}{2}\Delta\sigma(x) - \frac{|\nabla\sigma(x)|^2}{2} + V(x).$$

So we have the following essential equation:

$$\frac{|\nabla\sigma(x)|^2}{2} - V(x) = \frac{\hbar}{2}\Delta\sigma(x), \tag{4.8}$$

in which the left-hand side represents the *instanton Hamiltonian* and the right-hand side is the quantum viscosity term. Thus, we have obtained a viscous Hamilton-Jacobi equation that we have recalled in the general form (1.14) in Section 1.2. The only difference is that in the case above the potential appears with the minus sign. Precisely for this reason it is called Instanton Hamiltonian. [1]
We just remember that in Section 1.2 we have explored the general properties of the viscous equation and in particular we have enounced the main theorems about this topic proved by Gomes and Anantharaman [2, 17].

Using Theorem 4 with the viscosity coefficient $\hbar$ fixed, we have that there exists a unique constant $c(\hbar) \in \mathbb{R}$ such that the equation

$$\frac{|\nabla\sigma(x)|^2}{2} - V(x) = c(\hbar) + \frac{\hbar}{2}\Delta\sigma(x) \tag{4.9}$$

has a global viscosity solution, that we denote $\sigma_\hbar(x)$.
If we compute the semi-classical limit $\hbar \to 0$, we obtain

$$c(\hbar) \longrightarrow c[0],$$

[1] There is a rich literature of this inversion of the sign in front of the true potential: many authors used the so-called *Wick rotation*, see e.g. [15, 29]. We do not enter in this topic here.

that is exactly the Mañé critical value, and

$$\sigma_\hbar(x) \longrightarrow \sigma_0(x),$$

that is again a viscosity solution. So in this particular case the semi-classical limit is identified with a viscosity limit.

**Remark.** We can immediately observe that in the above example the Mañé critical value vanishes, in fact:

$$c[0] = \max_{x\in\mathbb{T}^n}(-V(x)) = \min_{x\in\mathbb{T}^n} V(x) = 0.$$

But the most important result in this quantum theory is that the solution $\sigma_\hbar(x)$ is *unique* up to constants. Also this fact is a consequence of Theorem 4.

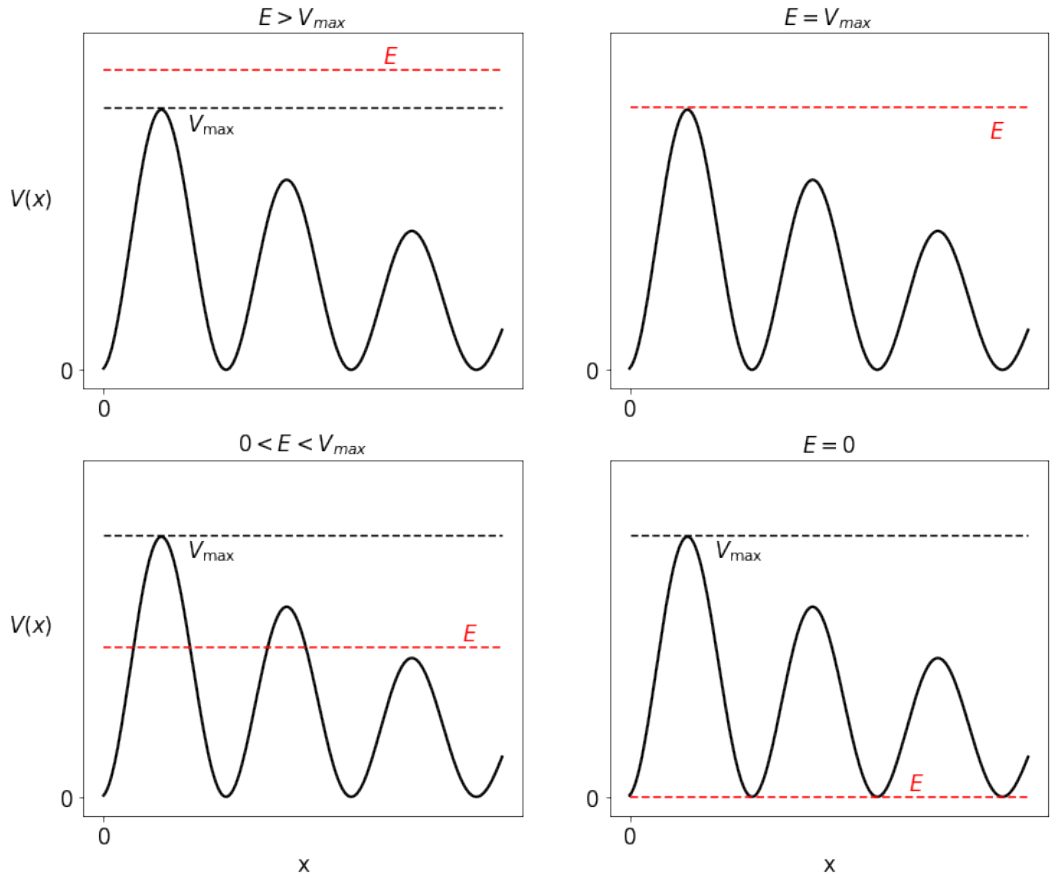


Figure 4.1: An example of bounded and continuous potential $V(x)$ and of the intervals taken into exam. For $E > V_{\max}$ there not exist any viscosity solution, but we have discovered that for the case $(i)$ such a solution exists only for the lower bound $E = V_{\max}$. For $0 < E < V_{\max}$ (case $(ii)$) we obtain oscillating WKB solutions and finally, in the case $(iii)$, we analyze the ground state $E = V_{\min} = 0$ and found out a well-defined and unique viscosity solution.

We have summarized the results found in Figure 4.1.
In the next section we will go on to investigate the properties of the wave function at the minimum level $E = 0$.

## 4.2 Ground state of multiple-well problem

Until now, we have seen that the uniqueness is a solid fact in our arguments even though we have to consider $c(\hbar) \neq 0$ for $\hbar \neq 0$.
In this section we want to explore more about the ground state wave function $\sigma_\hbar(x)$ and, in particular, we are interested in finding out innovative results about the multiple-well problem. To do this, we leverage the fixed point problem around the semi-group $T_t^-$, that we have already mentioned in the previous chapters.

**Remark.** The following considerations are independent of whether the minimum of the potential energy $V(x)$ will be realized in one, two or $k$ points.

Therefore, starting from the candidate structure (4.2), we have found that the wave function of the ground state has the form

$$\varphi_\hbar(x) = e^{-\frac{\sigma_\hbar(x)}{\hbar}},$$

where the real function $\sigma_\hbar(x)$ has to satisfy the following viscous Hamilton-Jacobi equation:

$$\frac{|\nabla \sigma_\hbar(x)|^2}{2} - V(x) = \frac{\hbar}{2}\Delta\sigma_\hbar(x).$$

In particular, we are interested to the semi-classical limit $\hbar \to 0$. We have seen in the previous section that $\sigma_0(x)$ is a viscosity solution of the stationary Hamilton-Jacobi equation

$$\frac{|\nabla \sigma(x)|^2}{2} - V(x) = c[0] \tag{4.10}$$

for $c[0] = 0$, that is precisely the maximum of the instanton potential energy $-V$.

We have reached the key point of our arguments.
Before proceeding, it is necessary to recall an essential theorem from Section 1.2. It is a result of Fathi and is presented in details in his preliminary version of the book [11].
It is a characterization for viscosity solutions.

**Theorem 22.** *The function $u$ is a viscosity solution of the stationary Hamilton-Jacobi equation $H(x, Du(x)) = c$ if and only if it solves the following fixed point problem:*
*for all $x \in \mathbb{T}^n$ and for all $t \geq 0$,*

$$u(x) = \inf_\gamma \left\{ u(\gamma(0)) + \int_0^t L(\gamma(s), \dot\gamma(s))ds \right\} + ct, \tag{4.11}$$

*where the inf is taken over all piecewise $C^1$ curves $\gamma : [0, t] \to \mathbb{T}^n$ such that $\gamma(t) = x$.*

The constant $c$ is precisely the Mañé critical value $c[0]$.

In light of this fundamental theorem, we can proceed with our considerations.
Since $\sigma_0(x)$ is a viscosity solution of the stationary equation (4.10), we can state from Theorem 22 that this function is a fixed point of

$$\sigma(x) = \inf_{\gamma} \left( \sigma(\gamma(0)) + \int_0^t \frac{|\dot{\gamma}(s)|^2}{2} + V(\gamma(s))ds \right) + c[0]t \tag{4.12}$$

or, equivalently, we have that

$$\sigma(x) = T_t^- \sigma(x) + c[0]t.$$

Here, $L = \frac{1}{2}|\dot{q}|^2 + V$ is precisely the instanton Lagrangian function and in our specific case the Mañé critical value vanishes, i.e. $c[0] = 0$.

In what follows our aim is to give an innovative interpretation to the fixed point equation (4.12).
We start recalling Proposition 2 due to Carmona-Simon [4], that provides an alternative definition of the Agmon metric:

$$\rho(x,y) = \inf_{\gamma,T} \left\{ \frac{1}{2} \int_0^T |\dot{\gamma}(s)|^2 ds + \int_0^T V(\gamma(s))ds | \, \gamma(0) = x, \, \gamma(T) = y \right\}$$

with $x, y \in \mathbb{T}^n$. In the proof we got the following calculations:

$$0 \leq \frac{1}{2} \left( |\dot{\gamma}(s)| - \sqrt{2V(\gamma(s))} \right)^2 = \frac{|\dot{\gamma}(s)|^2}{2} + V(\gamma(s)) - \sqrt{2V(\gamma(s))}|\dot{\gamma}(s)|,$$

that we can rewrite as

$$\sqrt{2V(\gamma(s))}|\dot{\gamma}(s)| \leq \frac{|\dot{\gamma}(s)|^2}{2} + V(\gamma(s)).$$

Moving to integrals, we obtain:

$$\int_0^T \sqrt{2V(\gamma(s))}|\dot{\gamma}(s)|ds \leq \int_0^T \left[ \frac{|\dot{\gamma}(s)|^2}{2} + V(\gamma(s)) \right] ds \tag{4.13}$$

and the inequality is preserved even passing to the inf.
In particular, the equality is achieved at the minimum energy level $E = 0$. Indeed, in that case we have

$$\frac{|\dot{\gamma}(s)|^2}{2} - V(\gamma(s)) = 0,$$

that means

$$|\dot{\gamma}(s)| = \sqrt{2V(\gamma(s))}.$$

We continue analyzing the relation (4.13).
The left-hand side represents an integral with Lagrangian

$$\mathcal{L}(\gamma, \dot{\gamma}) = \sqrt{2V(\gamma)}|\dot{\gamma}|,$$

called *Agmon Lagrangian*, defined in Section 1.3.
It is positively 1-homogeneous in the variable $\dot{\gamma}$, so it results invariant under reparametrization of the time:

$$\begin{aligned} [0, T] &\longrightarrow [0, 1] \\ s &\longmapsto \tau(s) := \frac{s}{T}. \end{aligned} \tag{4.14}$$

**Remark.** We note that at points where the potential energy $V$ vanishes, separating curves $\gamma$ cannot be reparametrized with *finite* times $T$ and an opportune procedure is needed. Thus, before reparametrizing, we shift the path with a change of arc length so that zeros of $V$ are avoided. See for more detail Section 1.3, after the proof of Proposition 2.

Using the parametrization (4.14), the left-hand integral of (4.13) become

$$\int_0^1 \sqrt{2V(\gamma(\tau))}|\dot{\gamma}(\tau)|d\tau, \tag{4.15}$$

where the curve $\gamma : [0, 1] \to \mathbb{T}^n$ is such that $\gamma(0) = x$, $\gamma(1) = y$.
If we consider the metric induced by the Lagrangian $\mathcal{L}(\gamma, \dot{\gamma})$, the stationary curves at level $E = 0$ are said *Agmon geodesics* and the integral

$$\rho(x, y) := \inf_{\gamma} \int_0^1 \sqrt{2V(\gamma(\tau))}|\dot{\gamma}(\tau)|d\tau, \tag{4.16}$$

with $\gamma : [0, 1] \to \mathbb{T}^n$ and $\gamma(0) = x, \gamma(1) = y$, is exactly the *Agmon metric*.

Using these last considerations, we are finally ready to rewrite the equation (4.12):

$$\sigma(x) = \inf_{\gamma} \left( \sigma(\gamma(0)) + \int_0^1 \sqrt{2V(\gamma(\tau))}|\dot{\gamma}(\tau)|d\tau \right), \tag{4.17}$$

where the inf is taken over all curves $\gamma : [0, 1] \to \mathbb{T}^n$ such that $\gamma(1) = x$.
We observe that we can give the following characterization for the *fixed point function* in the multiple-well case:

**Theorem 23.** *Let $a_1, a_2, .., a_k$ be the points of the torus $\mathbb{T}^n$ in which the potential vanishes, i.e. $V(a_\alpha) = 0$, for $\alpha = 1, .., k$.*
*Then the fixed point function is defined as*

$$\sigma(x) = \min \{\rho(a_1, x), \rho(a_2, x), ..., \rho(a_k, x)\}, \tag{4.18}$$

*where $\rho$ is the Agmon metric given in (4.16).*

*Proof.* It is just a simple check.
We suppose that in correspondence of a generic point $x$, the minimum of equation (4.18) is reached relatively to the well $a_i$. From the definition of the Agmon metric (4.16), we have that

$$\rho(a_i, x) = \inf_{\gamma} \int_0^1 \sqrt{2V(\gamma(\tau))} |\dot{\gamma}(\tau)| d\tau \tag{4.19}$$

with $\gamma(0) = a_i$ and $\gamma(1) = x$.
To conclude the proof, we observe that $\sigma(x) = \rho(a_i, x)$ solves equation (4.17), since

$$\sigma(\gamma(0)) = \sigma(a_i) = 0$$

and the very definition (4.16).

□

This theorem is the most important achievement of this thesis. We have been able to generalize the results found by Simon for the double wells to the more general case of a multiple-well problem on the torus. Another important aspect of our analysis is characterized by the use of modern techniques, such as viscosity solutions and weak KAM theory.

Lastly, we can also rewrite Theorem 7 found by Simon and proved using the differential equation methods of Agmon [1, 32, 34]. We always consider the multiple-well case.

**Theorem 24.** *For any $x \in \mathbb{T}^n$, we have that*

$$\lim_{\hbar \to 0} \{-\hbar \ln \varphi_\hbar(x)\} = \sigma(x), \tag{4.20}$$

*where the limit is uniform on compact subset of $x$.*

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