Università degli Studi di Padova

Dipartimento di Matematica

SCUOLA DI DOTTORATO DI RICERCA IN: MATEMATICA
INDIRIZZO: MATEMATICA
CICLO: XXIV

Semiclassical limit: coherent states, quasimodes and WKB approximation

Direttore della Scuola: Ch.mo Prof. Paolo Dai Pra

Coordinatore d'indirizzo: Ch.mo Prof. Franco Cardin

Supervisore: Ch.mo Prof. Franco Cardin

Dottorando: Simone Vazzoler

Contents

Introduction

In this work we want to enlight some special aspects and further possible connections between Quantum and Classical Mechanics. The problem of the realtion between Quantum Mechanics and Classical Mechanics (QM and CM from now on) has a long history which dates back to Einstein in 1917 ([Ein17]) and Schrödinger in 1926 ([Sch26]). This bond has been studied, mainly, using two different point of view: the first one is called *quantization* and the second one is the *semiclassical limit* or *de-quantization*.
In the first chapter, we reconsider a general setting for the Coherent States on $\mathbb{R}^n$. We start introducing the definition of Minimal Uncertainty STate (MUST), we derive the general form for these states and we propose an integral equation (1.2.2) (involving the convolution with a Gaussian) characterizing the phases of the MUSTs. Moreover, using Poisson Summation Formula and the periodization operator, we are able to treat Coherent States on the flat Torus $\mathbb{T}^n$. Then (in the spirit of [AAG00] and [Per86]) we introduce the Heisenberg-Weyl algebra and group and we show that the group action on the set of Gaussians creates precisely the set of Canonical Coherent States ($\mathfrak{S}_{CCS}$): the elements of $\mathfrak{S}_{CCS}$ satisfy the integral equation (1.2.2), furthermore, by looking closer to the convolution equation, we show that it does not admit more general solutions, at least among the polynomial functions on $\mathbb{R}$.
Next, we study the propagation of Gaussian Coherent States. We look at their time evolution. We elaborate some theorems concerning Gaussian Coherent State approximation and we put in evidence that the approximate solutions behave in very different ways depending strongly on the possible stability character of the point on which the initial states are centered. But there is a common behaviour: every coherent state, centered on an unstable equilibrium point, starts spreading exponentially fast (at a rate given by the Lyapunov exponent) around the unstable manifold. By this line of thought, we restore some interesting statements by Paul proposed in [Pau07b]and [Pau09]. In the last part of this chapter we look at the Wick rotation: we propose some possible connections between approximate solutions of real Schrödinger equation, the work of Iturriaga in [ISM09], the work of Davini and Siconolfi [DS06] and more generally with WKAM theory. The references for this part are [CR97], [Pau07a], [Pau09], [Rob98], [Rob07] and [Sch01].
In the second chapter, we study Quasimodes for standard (i.e. mechanical) stationary Schrödinger operators in $\mathbb{T}^n$. In the beginning we follow the paper of Evans [Eva07], in which the author constructs a quasimode (with discrepancy $O(\varepsilon)$) from a variational principle. Then, in order

to construct quasimodes, we propose some applications of WKB approximation on the line of thought of Hellfer, see [Hel88]. Then, inspired by Lazutkin's techniques [Laz93] and with a particular choice of the couple energy-amplitude, we are able to recover one result of Evans: more precisely, we prove that the Effective Quantum Hamiltonian $\bar{H}_\varepsilon(P)$ coincides in $P = 0$, up to second order terms, with the WKB energy $E(\varepsilon)$ we have constructed.
In chapter three we start studying the evolutive Schrödinger equation for the Schwartz kernel using Fourier Integral Operators (FIO). Using this approach we show that it is possible to approximate the solution up to a fixed time T at which the caustics (of the associated Hamilton-Jacobi equation) appear. We see that the first order terms are nothing but a system of PDEs given by an Hamilton-Jacobi and a transport equation. We show that is possible to overcome this difficulty using the group property of the FIOs: here we suggest a connection with the Symplectic Homogenization presented in [Vit08]. Then we change the point of view and we start looking at the so called "Madelung equations". Solutions for this system of PDEs are not easy write down (even in a weak environment) and so perform an approximation on these equations by considering again the WKB setting. In the last part we modify the Madelung equations to obtain two different systems of PDEs corresponding to nonlinear Schrödinger equations and in this cases we found the stationary solutions.
Next, in the fourth chapter, Aubry-Mather's and Weak KAM theory are presented. Here we propose some connections among these subjects and results perfomed in the previous chapters: we look for conditions on the classical Hamiltonian that give the uniqueness for the solution of the stationary Hamilton-Jacobi equation

$$H(x, \nabla S) = E$$

In this part we follow Anantharaman and others, [AIPSM05]: we emphasize in particular that, under certain assumptions, the unique solution of this equation is a generating function (in a weak sense) of the unstable manifold. In the last part of this chapter we try to underline the possible connections between our work and Quantum Unique Ergodicity (QUE).

Introduzione

In questo lavoro si vogliono mettere in luce alcuni aspetti ed alcune connessioni tra la Meccanica Classica e la Meccanica Quantistica. Il problema della relazione tra Meccanica Quantistica e Meccanica Classica (QM e CM d'ora in poi) ha una lunga storia il cui inizio puó essere fatto risalire ad Einstein nel 1917 ([Ein17]) e Schrödinger nel 1926 ([Sch26]). Questo legame è stato studiato, principalmente, usando due punti di vista differenti ed opposti: il primo è detto *quantizzazione* ed il secondo *limite semiclassico* o *de-quantizzazione*.
Nel primo capitolo vengono introdotti gli Stati Coerenti su $\mathbb{R}^n$. Partendo dalla definizione di Minimal Uncertainty STates (stati quantistici ad incertezza minima o MUSTs), si ricava la forma generale di questi stati e si propone un'equazione integrale (si veda l'equazione (1.2.2)) che descrive la fase di ogni MUST. Inoltre, usando la formula di Poisson e l'operatore di periodizzazione, si mostra che è possibile definire gli Stati Coerenti anche sul toro piatto $\mathbb{T}^n$. Seguendo le idee di Ali, Antoine e Gazeau in [AAG00] e Perelomov in [Per86] vengono definiti ed introdotti l'algebra e il gruppo di Heisenberg-Weyl. Succesivamente si mostra che l'azione di tale gruppo sull'insieme delle Gaussiane genera esattamente l'insieme degli Stati Coerenti Canonici ($\mathfrak{S}_{CCS}$): gli elementi di tale insieme soddisfano l'equazione (1.2.2) ed inoltre, esaminando in maggior dettaglio l'equazione stessa, si mostra che essa non ammette soluzioni più generali (almeno nella classe dei polinomi su $\mathbb{R}$).
Successivamente viene studiata la propagazione degli Stati Coerenti Gaussiani. Guardando alla loro evoluzione temporale, vengono elaborati alcuni teoremi riguardanti l'approsimazione mediante Stati Coerenti e viene messo in evidenza che il comportamento della soluzione approssimata dipende fortemente dalla stabilità (o instabilità) del punto dello spazio delle fasi classico in cui lo Stato Coerente è centrato. È però importante notare che vi è un comportamento comune: ogni Stato Coerente, centrato in punto di equilibrio instabile, si "disperde" con una velocità esponenziale (e legata all'esponente di Lyapunov del punto) attorno alla varietà instabile. In questo modo vengono ritrovati i risultati annunciati da Paul in [Pau07b] e [Pau09]. Nell'ultima parte del primo capitolo si studiano la rotazione di Wick e l'equazione di Schrördinger reale: vengono messi in evidenza alcuni legami tra le soluzioni approssimate dell'equazione di Schrödinger reale e i lavori di Iturriaga [ISM09] e Davini e Siconolfi [DS06].
Nel secondo capitolo vengono studiati i quasimodi per gli operatori di Schrödinger meccanici su $\mathbb{T}^n$. Nella prima parte del capitolo si segue il lavoro di Evans [Eva07], in cui l'autore

riesce a costruire un quasimodo (con discrepanza $O(\varepsilon)$) partendo da un principio variazionale. Successivamente vengono proposte e richiamate alcune applicazioni della teoria WKB nella costruzione di quasimodi seguendo quanto fatto da Hellfer in [Hel88] e poi, ispirandosi ai lavori di Lazutkin in [Laz93] e segliendo una particolare coppia energia-ampiezza di probabilità, si mostra che è possibile ritrovare un risultato di Evans: più precisamente si mostra che l'Hamiltoniana Effettiva Quantistica $\bar{H}_\varepsilon(P)$ coincide in $P = 0$, fino ai termini del secondo ordine, con l'energia $E(\varepsilon)$ costruita con i metodi WKB.
Nel terzo capitolo si studia l'equazione di Schrödinger evolutiva per il nucleo di Schwartz, usando gli operatori integrali di Fourier (FIO). Usando questo metodo si mostra che è possibile approssimare la soluzione fino ad un tempo T fissato in cui appaiono le caustiche (relative all'equazione di Hamilton-Jacobi associata). I termini del primo ordine di quest'approssimazione sono un sistema di PDE costituito da un equazione di Hamilton-Jacobi e un'equazione del trasporto: si mostra che è possibile superare il problema delle caustiche sfruttando la proprietà di gruppo degli operatori integrali di Fourier: in questa parte si suggerisce un possibile collegamento con l'omogeneizzazione simplettica sviluppata da Viterbo in [Vit08]. Successivamente si cambia punto di vista e si studiano le equazioni di Madelung: non è possibile scrivere esplicitamente una soluzione di queste equazioni (nemmeno soluzioni deboli); per questo motivo si cerca una soluzione approssimata del sistema di equazioni considerando, ancora una volta, un'approssimazione WKB. Nell'ultima parte del capitolo vengono modificate le equazioni di Madelung per ottenere due differenti sistemi di PDE corrispondenti a delle equazioni di Schrödinger non lineari e in questi casi è possibile trovare una soluzione stazionaria (anche questa volta la soluzione è legata alla teoria WKAM).
Infine nell'ultimo capitolo vengono introdotte le teorie classiche WKAM e di Aubry-Mather. Qui si propongono delle connessioni tra questi argomenti e i risultati dei precedenti capitoli: si cercano delle condizioni sull'Hamiltoniana classica che diano l'unicità della soluzione dell'equazione di Hamilton-Jacobi stazionaria

$$H(x, \nabla S) = E$$

In questa parte si segue principalmente Anantharaman e altri in [AIPSM05]: sotto alcune condizioni sul potenziale, l'unica soluzione di tale equazione, descrive localmente la varietà instabile.

Ringraziamenti

Ringrazio i Professori Andrea Sacchetti e Franco Cardin per l'aiuto e i suggerimenti che mi hanno fornito durante la stesura di questo lavoro. In particolare voglio ringraziare il Prof. Sacchetti per l'ospitalità dimostrata durante i giorni trascorsi a Modena.
Tutte le cose che capirete dopo aver letto questa tesi sono merito loro, quelle che non riuscirete a capire sono solo merito mio.

Un ringraziamento speciale va anche alla mia famiglia (ai miei genitori Ivano e Gigliola, a Cristiano, Emanuele e Serena, Orso), a tutti i miei parenti e amici per avermi sostenuto e soprattutto sopportato durante questi anni.

Chapter 1

Coherent States and their evolution

The problem of understanding the relation between Classical and Quantum Mechanics has a long history which dates back to Schrödinger in 1926 when he constructed minimum uncertainty wave packets for the harmonic oscillator (see [Sch26]).
Before starting we make some remarks on the environments we will be working on: all Hilbert spaces $\mathcal{H}$ we consider will be complex and separable ($\dim \mathcal{H}$ will be countably infinite). Moreover the scalar product will be indicated by $\langle \phi, \psi \rangle$ or $\langle \phi | \psi \rangle$ and will be antilinear in the first variable ϕ and linear in the second ψ. We will use capital letters for the operators on $\mathcal{H}$ and small letters for the functions (for example: if h is an Hamiltonian function then H will be its corresponding operator on the Hilbert space). Here we will follow [AAG00], [Pau07b], [Pau07a], [Pau09].
About the notations: throughout all this work ε will represent the Planck's constant $\hbar$.

1.1 Quantum Mechanics

In this section we will introduce the general setting of Quantum Mechanics (QM from now on) and we will explain all the notation we will use.
In QM the state of a physical system is described by a complex-valued function ψ (also called wave function) that belongs to an Hilbert space $\mathcal{H}$. Tipically we will consider

$$\mathcal{H} = L^2(\mathbb{R}^n) = \left\{ \psi : \mathbb{R}^n \to \mathbb{C} : \int_{\mathbb{R}^n} \psi^*(x)\psi(x)dx < +\infty \right\}$$

We will use also the bra-ket notation: in this case the state $\psi(x)$ will be described by the vector $|\psi\rangle$ of the Hilbert space $\mathcal{H}$ and the scalar product on $\mathcal{H}$ will be given by

$$\langle \phi | \psi \rangle = \int_{\mathbb{R}^n} \phi^*(x)\psi(x)dx$$

Quantum observables are described by self-adjoint (or essentially self-adjoint) operators acting on the Hilbert space $\mathcal{H}$. We will use capital letters for operators: for example the action of the operator A on the state ψ will be given by $A\psi$ or, using bra and ket, by $|A\psi\rangle$.

Definition 1.1.1. *Let $\mathcal{H}$ an Hilbert space. An operator $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ where $D(A)$ is the domain of A, is symmetric if*

$$\langle Ax|y\rangle = \langle x|Ay\rangle \tag{1.1.1}$$

for all $x, y \in D(A)$.

Before giving the definition of self-adjoint operator, we have to define the adjoint $A^\dagger$ of an operator A.

Definition 1.1.2. *Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ a densely defined linear operator. The adjoint $A^\dagger$ of A is defined in the following way.*

(a) The domain $D(A^\dagger)$ is the subset of $\mathcal{H}$ that contains all the vector x such that

$$y \mapsto \langle x|Ay\rangle$$

is a continuous linear functional. Since it is continuous and densely defined it can be extended to a continuous linear functional on all of $\mathcal{H}$.

(b) If x is in $D(A^\dagger)$, then there exists an unique element $z \in \mathcal{H}$ such that

$$\langle x|Ay\rangle = \langle z|y\rangle \tag{1.1.2}$$

for all $y \in D(A)$.

The vector z is defined to be $A^\dagger x$.

Note that the adjoint operator is well well defined, using the denseness of the domain of the operator and the uniqueness of Riesz representation (point (b)).

Definition 1.1.3. *Let A be an operator densely defined on $\mathcal{H}$. A is self-adjoint if $A = A^\dagger$ and $D(A) = D(A^\dagger)$. We will say that A is essentially self-adjoint if A is self-adjoint and it admits an unique self-adjoint extension to $\mathcal{H}$.*

The outcome of measuring an observable A is given by the mean value of the operator A on the state ψ and will be denoted by

$$\langle A\rangle_\psi = \langle\psi|A\psi\rangle = \int_{\mathbb{R}^n} \psi^*(x)A\psi(x)dx$$

The two most important operators that we will use in the following are $(X_i\psi)(x) = x_i\psi(x)$ (the multiplication operator) and $(P_i\psi)(x) = -\mathrm{i}\varepsilon\partial_{x_i}\psi(x)$ (the momentum operator). Both X and P are self adjoint operators with domains

$$D(X) = \{\psi \in \mathcal{H} \,|\, x_k\psi \in \mathcal{H},\ \forall k = 1, \dots, n\}$$
$$D(P) = \{\psi \in \mathcal{H} \,|\, \partial_{x_k}\psi \in \mathcal{H},\ \forall k = 1, \dots, n\}$$

The operators X and P satisfy the canonical commutation relations (also called Heisenberg commutation relation)

$$[X_i, P_j] = \mathrm{i}\varepsilon\delta_{ij}I \tag{1.1.3}$$

where the brackets represent the commutator and are defined as $[A, B] := AB - BA$ on the domain of $X \cdot P - P \cdot X$.

Theorem 1.1.4. *Equation (1.1.3) implies that for any vector ψ sufficiently smooth, with $\|\psi\|_{L^2(\mathbb{R}^n)} = 1$, the Heisenberg uncertainty relations hold:*

$$(\Delta X_i)_\psi (\Delta P_i)_\psi \geq \frac{\varepsilon}{2} \tag{1.1.4}$$

for $i = 1, \ldots, n$, where for an arbitrary self-adjoint operator A on $\mathcal{H}$

$$(\Delta A)_\psi = \sqrt{\langle\psi|A^2\psi\rangle - \langle\psi|A\psi\rangle^2}$$

Proof. We start from Schwartz inequality: for every couple of operators A and B and for every state $\psi(x)$ with $\|\psi\|_{L^2(\mathbb{R}^n)} = 1$ one has

$$\langle A^2\rangle_\psi\langle B^2\rangle_\psi = \int_{\mathbb{R}^n}(A\psi)^*(A\psi)dx\int_{\mathbb{R}^n}(B\psi)^*(B\psi)dx \geq \left|\int_{\mathbb{R}^n}(A\psi)^*(B\psi)dx\right|^2 = \left|\int_{\mathbb{R}^n}\psi^*A(B\psi)dx\right|^2$$

We can write

$$\int_{\mathbb{R}^n}\psi^*A(B\psi)dx = \frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB+BA)\psi dx + \frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB-BA)\psi dx$$

and thus

$$\langle A^2\rangle_\psi\langle B^2\rangle_\psi \geq \left|\frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB+BA)\psi dx + \frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB-BA)\psi dx\right|^2$$

Now, since the expected value of the operator $\frac{AB+BA}{2}$ is real while the expected value of $\frac{AB-BA}{2}$ is purely imaginary, we have that

$$\begin{aligned}&\left|\frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB+BA)\psi dx + \frac{1}{2}\int_{\mathbb{R}^n}\psi^*(AB-BA)\psi dx\right|^2 = \\ &= \frac{1}{4}\left|\int_{\mathbb{R}^n}\psi^*(AB+BA)\psi dx\right|^2 + \frac{1}{4}\left|\int_{\mathbb{R}^n}\psi^*(AB-BA)\psi dx\right|^2\end{aligned}$$

and since $\frac{1}{4}\left|\int_{\mathbb{R}^n}\psi^*(AB+BA)\psi dx\right|^2 \geq 0$ we can write

$$\langle A^2\rangle_\psi\langle B^2\rangle_\psi \geq \frac{1}{4}\left|\int_{\mathbb{R}^n}\psi^*[A,B]\psi dx\right|^2$$

Now we make the substitution $A = \Delta X_i$ and $B = \Delta P_i$, using (1.1.3) and the fact that

$\langle(\Delta X_i)^2\rangle_\psi = (\Delta X_i)^2_\psi$ and $\langle(\Delta P_i)^2\rangle_\psi = (\Delta P_i)^2_\psi$, we have

$$(\Delta X_i)^2_\psi(\Delta P_i)^2_\psi \geq \frac{\varepsilon^2}{4}$$

that implies (1.1.4). □

1.2 Coherent States

We start searching on the Hilbert space $L^2(\mathbb{R}^n)$ for the "most classical" states of QM.

Definition 1.2.1. *The wave function $\psi(x)$ is a coherent state (or MUST: Minimal Uncertainty STate) if*

$$(\Delta X_i)_\psi(\Delta P_i)_\psi = \frac{\varepsilon}{2}$$

The next step is to find the general form for a coherent state on $\mathbb{R}^n$ since the previous definition tells us nothing about it. For a MUST we propose the following characterization for the amplitude and the phase.

Proposition 1.2.2. *A coherent state $\eta_{(q,p)}(x)$ has the following representation*

$$\eta_{(q,p)}(x) = \left(\frac{1}{\pi\varepsilon}\right)^{n/4} e^{\frac{\mathrm{i}}{\varepsilon}\varphi_{(q,p)}(x)} \prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{2\varepsilon}}$$

where $\partial_{x_i}\varphi_{(q,p)}$ solves

$$\left\langle \eta \middle| (\partial_{x_i}\varphi_{(q,p)})^2\eta \right\rangle - \left\langle \eta \middle| \partial_{x_i}\varphi_{(q,p)}\eta \right\rangle^2 = 0 \tag{1.2.1}$$

The last equation can be rewritten as

$$\left[(\partial_{x_i}\varphi_{(q,p)})^2 * \mathcal{G}\right](q) = \left[\partial_{x_i}\varphi_{(q,p)} * \mathcal{G}\right]^2(q) \tag{1.2.2}$$

with

$$\mathcal{G}(x) = \left(\frac{1}{\pi\varepsilon}\right)^{n/2} \prod_{i=1}^{n} e^{-\frac{x_i^2}{\varepsilon}}$$

and $*$ indicates the convolution.

Proof. We will have

$$(\Delta X_i)_\eta(\Delta P_i)_\eta = \frac{\varepsilon}{2}$$

when

$$|\langle X_i\eta|P_i\eta\rangle| = |X_i\eta|^2|P_i\eta|^2$$

i.e. when $X_i\eta$ and $P_i\eta$ are parallel vectors. This means, in particular, that

$$-\mathrm{i}\varepsilon\partial_{x_i}\eta(x) = \alpha x_i \eta(x)$$
$$\eta(x) = C\prod_{i=1}^{n} e^{\mathrm{i}\alpha_i \frac{x_i^2}{2\varepsilon}}$$

where C is the normalization constant such that

$$\int_{\mathbb{R}^n} |\eta(x)|^2\, dx = 1$$

Since η must be in $\mathcal{H} = L^2(\mathbb{R}^n, dx)$, we must have $\alpha_i \in \operatorname{Im}\mathbb{C}_{>0}$ for every i. So a coherent states must have the following form:

$$\eta_{(q,p)}(x) = \frac{1}{(\pi\varepsilon)^{n/4}} e^{\frac{i}{\varepsilon}\varphi_{(q,p)}(x)} \prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{2\varepsilon}}$$

Now we want to find the equation satisfied by $\varphi_{(q,p)}(x)$. It is easy to see that

$$(\Delta X_i)_{\eta_{(q,p)}} = \sqrt{\frac{\varepsilon}{2}}$$

that means we must have

$$(\Delta P_i)_{\eta_{(q,p)}} = \sqrt{\frac{\varepsilon}{2}}$$

Using the following equalities

$$P_i\eta_{(q,p)} = \left[\mathrm{i}(x_i - q_i) + \partial_{x_i}\varphi_{(q,p)}(x)\right]\eta_{(q,p)}(x)$$
$$P_i^2\eta_{(q,p)} = \left[\varepsilon - \mathrm{i}\varepsilon\partial_{x_i}^2\varphi_{(q,p)}(x) + \left(\mathrm{i}(x_i - q_i) + \partial_{x_i}\varphi_{(q,p)}(x)\right)^2\right]\eta_{(q,p)}(x)$$
$$\left\langle \eta_{(q,p)} \middle| P_i\eta_{(q,p)} \right\rangle^2 = \left[C(\varepsilon)\int_{\mathbb{R}^n} \partial_{x_i}\varphi_{(q,p)}(x) \prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{\varepsilon}} dx\right]^2$$
$$\left\langle \eta_{(q,p)} \middle| P_i^2\eta_{(q,p)} \right\rangle = \frac{\varepsilon}{2} + C(\varepsilon)\int_{\mathbb{R}^n} (\partial_{x_i}\varphi_{(q,p)}(x))^2 \prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{\varepsilon}} dx$$

Now we compute

$$\begin{aligned}\left\langle \eta_{(q,p)} \middle| P_i\eta_{(q,p)} \right\rangle &= \mathrm{i}\left\langle \eta_{(q,p)} \middle| (x_i - q_i)\eta_{(q,p)} \right\rangle + \left\langle \eta_{(q,p)} \middle| \partial_{x_i}\varphi_{(q,p)}(x)\eta_{(q,p)}(x) \right\rangle \\ &= \left\langle \eta_{(q,p)} \middle| \partial_{x_i}\varphi_{(q,p)}(x)\eta_{(q,p)}(x) \right\rangle\end{aligned}$$

since $\left\langle \eta_{(q,p)} \middle| (x_i - q_i)\eta_{(q,p)} \right\rangle = 0$ (it is the first central moment of a Gaussian). In the same way

$$\begin{aligned}
\left\langle \eta \middle| P_i^2 \eta \right\rangle &= \left\langle \eta \middle| \left[\varepsilon - \mathrm{i}\varepsilon\partial_{x_i}^2\varphi(x) + \Big(\mathrm{i}(x_i - q_i) + \partial_{x_i}\varphi(x)\Big)^2 \right] \eta \right\rangle \\
&= \varepsilon + \left\langle \eta \middle| (\partial_{x_i}\varphi)^2\eta \right\rangle - \left\langle \eta \middle| (x_i - q_i)^2\eta \right\rangle + \mathrm{i}\left(2\left\langle \eta \middle| (x_i - q_i)\partial_{x_i}\varphi\eta \right\rangle - \varepsilon\left\langle \eta \middle| (\partial_{x_i}^2\varphi)\eta \right\rangle\right) \\
&= \varepsilon + \left\langle \eta \middle| (\partial_{x_i}\varphi)^2\eta \right\rangle - \frac{\varepsilon}{2} + \mathrm{i}\left(2\left\langle \eta \middle| (x_i - q_i)\partial_{x_i}\varphi\eta \right\rangle - \varepsilon\left\langle \eta \middle| (\partial_{x_i}^2\varphi)\eta \right\rangle\right) \\
&= \frac{\varepsilon}{2} + \left\langle \eta \middle| (\partial_{x_i}\varphi)^2\eta \right\rangle + \mathrm{i}\left(2\left\langle \eta \middle| (x_i - q_i)\partial_{x_i}\varphi\eta \right\rangle - \varepsilon\left\langle \eta \middle| (\partial_{x_i}^2\varphi)\eta \right\rangle\right)
\end{aligned}$$

since $\left\langle \eta \middle| (x_i - q_i)^2\eta \right\rangle = \frac{\varepsilon}{2}$, being the second central moment of the Gaussian. Requiring that

$$\left\langle \eta \,\middle|\, \left[2(x_i - q_i)\partial_{x_i}\varphi_{(q,p)}(x) - \varepsilon\partial_{x_i}^2\varphi_{(q,p)}(x)\right] \eta \right\rangle = 0$$

(i.e. the imaginary part must be zero that is the second equation of (1.2.1)), it follows that

$$\langle \eta | P_i^2 \eta \rangle - (\langle \eta | P_i \eta \rangle)^2 = \frac{\varepsilon}{2} + \langle \eta | (\partial_{x_i}\varphi)^2 \eta \rangle - (\langle \eta | \partial_{x_i}\varphi\eta \rangle)^2$$

In order to have $\langle \eta | P_i^2 \eta \rangle - (\langle \eta | P_i \eta \rangle)^2 = \frac{\varepsilon}{2}$, we must require

$$\left\langle \eta_{(q,p)}(x) \middle| (\partial_{x_i}\varphi_{(q,p)}(x))\eta_{(q,p)}(x) \right\rangle - \Big(\left\langle \eta_{(q,p)}(x) \middle| (\partial_{x_i}\varphi_{(q,p)}(x))\eta_{(q,p)}(x) \right\rangle\Big)^2 = 0$$

and this equation implies that $\varphi_{(q,p)}(x)$ must satisfy the following equation

$$\int_{\mathbb{R}^n} (\partial_{x_i}\varphi_{(q,p)}(x))^2 \left(C(\varepsilon) \prod_{i=1}^n e^{-\frac{(x_i - q_i)^2}{\varepsilon}} \right) dx = \left[\int_{\mathbb{R}^n} \partial_{x_i}\varphi_{(q,p)}(x) \left(C(\varepsilon) \prod_{i=1}^n e^{-\frac{(x_i - q_i)^2}{\varepsilon}} \right) dx \right]^2$$

that is, defining

$$\mathcal{G}(x) = C(\varepsilon) \prod_{i=1}^n e^{-\frac{x_i^2}{\varepsilon}}$$

we have

$$\left[(\partial_{x_i}\varphi_{(q,p)})^2 * \mathcal{G} \right](q) = \left[\partial_{x_i}\varphi_{(q,p)} * \mathcal{G} \right]^2 (q)$$

which is exactly (1.2.2). $\square$

Remark 1.2.3 We make an example: take $\mathcal{H} = L^2(\mathbb{R}, dx)$. Then the simplest function $f(x)$ that satisfies the equation

$$\left[f^2 * \mathcal{G}\right](q) = [f * \mathcal{G}]^2 (q)$$

is $f(x) = p$, where $p \in \mathbb{R}$. Infact we have

$$p^2 \int_{\mathbb{R}} C(\varepsilon) e^{-\frac{(x-q)^2}{\varepsilon}} dx = \left[p \int_{\mathbb{R}} C(\varepsilon) e^{-\frac{(x-q)^2}{\varepsilon}} dx\right]^2$$

and thus the phase is $\varphi_{(q,p)}(x) = px + k$, where $k \in \mathbb{R}$ is a constant. Note that the same argumet can be applied in the n-dimensional case: if $\mathcal{H} = L^2(\mathbb{R}^n, dx)$ then the simplest function that satisfies (1.2.2) is $\varphi_{(q,p)}(x) = p \cdot x + k$ with $p \in \mathbb{R}^n$ and $k \in \mathbb{R}$. We will see in the following section that the right choice for k is $k = pq/2$.

Remark 1.2.4 Once we have found n functions f_i satisfying (1.2.2) it is necessary to find a function $\varphi_{(q,p)}$ such that

$$d\varphi_{(q,p)}(x) = \sum_{i=1}^{n} f_i(x) dx_i$$

globally. This means that the $f_i(x)$'s must be the components of a differential 1-form. On $\mathbb{R}^n$ there is the well known condition

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial f_j}{\partial x_i}$$

i.e. the functions must satisfy the closure condition in order to $\varphi_{(q,p)}(x)$ to exist. It is clear that the solution of the problem depends on the topology of the manifold M we are working on. In particular it depends on $H^1_{DR}(M)$, the first De Rham cohomology group of M (see [BT95] for details). For example, from the fact that $H^1_{DR}(\mathbb{R}^n) = 0$ and $H^1_{DR}(\mathbb{T}^n) \neq 0$ the solutions on these two manifolds will be different. It would be interesting also to understand if the definition (1.2.3) contains all the possible solutions to (1.2.1).

In $\mathbb{R}^n$ there exist a larger family of functions, called *Gaussons* or *Gaussian pure states*, that, for particular choices of the parameters, are similar to the MUST.

Definition 1.2.5. *The Gaussons have the following form (see [AAG00]):*

$$\eta^{U,V}_{(q,p)}(x) = \left(\frac{\det U}{\pi^n}\right)^{1/4} \exp\left[\frac{\mathrm{i}}{\varepsilon}\left\langle p, x - \frac{q}{2}\right\rangle\right] \exp\left[-\frac{1}{2}\left\langle x - q, (U + \mathrm{i}V)(x - q)\right\rangle\right] \tag{1.2.3}$$

where $x \in \mathbb{R}^n$, $(q,p) \in \mathbb{R}^{2n}$, U is a real $n \times n$ positive definite matrix and $V \in M_{n\times n}(\mathbb{R})$. We *will use the simbol $\mathfrak{S}_G$ to denote the set of Gaussons.*

When U is a diagonal matrix but not the identity matrix, these states are called *squeezed states.* If we write down explicitly the phase, we get

$$\varphi_{(q,p)}(x) = \left\langle p, x - \frac{q}{2} \right\rangle - \frac{1}{2}\langle x - q, V(x-q)\rangle \tag{1.2.4}$$

where V is an $n \times n$ matrix.

It is also possible to define *generalized* coherent states choosing as amplitude a more general function than the Gaussian as Paul did in [Pau09], but he consider as phase only the function $\varphi_{(q,p)}(x) = \langle p, x\rangle$ (plane wave). Here we extend his definition letting the phase be as in (1.2.4) for the gaussons.

Definition 1.2.6. *Let $a \in \mathcal{S}(\mathbb{R}^n)$ and $(q,p) \in \mathbb{R}^{2n}$. We define a generalized coherent state centered in (q,p) as the following wave function*

$$\psi^{a,V}_{(q,p)}(x) = a\left(\frac{x-q}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}\left(\langle p, x-q\rangle - \frac{1}{2}\langle V(x-q),(x-q)\rangle\right)} \tag{1.2.5}$$

where $\|a\|_{L^2} = 1$ and V is a real $n \times n$ matrix.

We want to underline that this type of Coherent States will be useful in the following sections when we will perform a semiclassical approximation of the solution of the Schrödinger equation. More precisely we will see that choosing as initial datum a Coherent State, it will evolve to a generalized Coherent State as in the previous definition.

1.2.1 On the convolution equation

Now we consider the convolution equation (1.2.2) in a more general form. In particular we assume that the variance σ of the Gaussian will take values in the interval $]0, +\infty[$. So the equation will take the form

$$\int_{\mathbb{R}^n} (\partial_{x_i}\varphi_{(q,p)}(x))^2 \left(C(\sigma)\prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{\sigma}}\right) dx = \left[\int_{\mathbb{R}^n} \partial_{x_i}\varphi_{(q,p)}(x)\left(C(\sigma)\prod_{i=1}^{n} e^{-\frac{(x_i-q_i)^2}{\sigma}}\right) dx\right]^2$$

In $\mathbb{R}$ this equation becomes

$$\int_{\mathbb{R}} (f_{(q,p)}(x))^2 \left(C(\sigma)e^{-\frac{(x-q)^2}{\sigma}}\right) dx = \left[\int_{\mathbb{R}} f_{(q,p)}(x)\left(C(\sigma)e^{-\frac{(x-q)^2}{\sigma}}\right) dx\right]^2 \tag{1.2.6}$$

and we will look for solutions of the form

$$f(x) = \sum_{i=0}^{d} a_i (x-q)^i$$

where $f:\mathbb{R}\to\mathbb{R}$ and $d=\deg f$ is the degree of the polynomial. Using this particular form for the solution f, we have that the integral on the right side of (1.2.6) is

$$\begin{aligned}\int_{\mathbb{R}} f_{(q,p)}(x)\left(C(\sigma)e^{-\frac{(x-q)^2}{\sigma}}\right)dx &= \sum_{i=0}^{d} a_i\left(C(\sigma)\int_{\mathbb{R}}(x-q)^i e^{-\frac{(x-q)^2}{\sigma}}dx\right)\\ &= \sum_{i=0}^{d} a_i\mathbb{E}[(N(q,\sigma)-q)^i]\end{aligned}$$

where $\mathbb{E}[(N(q,\sigma)-q)^i]$ stands for the central momentum of i-th order of the Normal distribution with mean q and variance σ. It is a well known fact that

$$\mathbb{E}[(N(q,\sigma)-q)^i]=\begin{cases}0 & \text{if } i \text{ is odd}\\ \sigma^i(i-1)!! & \text{if } i \text{ is even}\end{cases} \tag{1.2.7}$$

so that we have

$$\int_{\mathbb{R}} f_{(q,p)}(x)\left(C(\sigma)e^{-\frac{(x-q)^2}{\sigma}}\right)dx = \sum_{\substack{i=0\\ i\ \text{even}}}^{d} \sigma^i(i-1)!!a_i$$

Now

$$(f(x))^2=\sum_{i,j=0}^{d} a_i a_j (x-q)^{i+j}$$

and

$$\int_{\mathbb{R}} (f_{(q,p)}(x))^2\left(C(\sigma)e^{-\frac{(x-q)^2}{\sigma}}\right)dx = \sum_{\substack{i,j=0\\ i+j\ \text{even}}}^{d} \sigma^{i+j}(i+j-1)!!a_i a_j$$

so that equation (1.2.6) becomes

$$\sum_{\substack{i,j=0\\ i+j\ \text{even}}}^{d} \sigma^{i+j}(i+j-1)!!a_i a_j - \sum_{\substack{i,j=0\\ i,j\ \text{even}}}^{d} \sigma^{i+j}(i-1)!!(j-1)!!a_i a_j = 0 \tag{1.2.8}$$

To make things easier let us make some examples.

$d=1$

We are looking for a function f of the form

$$f(x)=a_0+a_1(x-q)$$

and equation (1.2.8) becomes

$$a_0^2+\sigma^2a_1^2-a_0^2=\sigma^2a_1^2=0$$

that implies $a_1 = 0$ and $a_0 = p \in \mathbb{R}$. This means, in particular, that the phase will be $\varphi_{(q,p)}(x) = p(x-q)$.

$d = 2$

Again

$$f(x) = a_0 + a_1(x-q) + a_2(x-q)^2$$

and (1.2.8) will take the form

$$a_0^2 + 2\sigma^2 a_0 a_2 + \sigma^2 a_1^2 + 3\sigma^4 a_2^2 - a_0^2 - 2\sigma^2 a_0 a_2 - \sigma^4 a_2^2 = a_1^2 + 2\sigma^2 a_2^2 = 0$$

and one has $a_0 = p \in \mathbb{R}_{>0}$ and $a_1 = a_2 = 0$.

To understand better we simply rewrite (1.2.8) in the following way

$$\sum_{\substack{i,j=0\\ i,j \text{ odd}}}^{d} \sigma^{i+j}(i+j-1)!!a_i a_j + \sum_{\substack{i,j=0\\ i,j \text{ even}}}^{d} \sigma^{i+j}[(i+j-1)!! - (i-1)!!(j-1)!!]a_i a_j = 0 \tag{1.2.9}$$

It is easy to see that this equation does not admit any solution different from $a_0 = p$ and $a_k = 0$ for $k = 1, \dots, d$. This means in particular, that the only real solution $\varphi(x)$ to the convolution equation of the form $\partial_{x_i}\varphi(x) = f_i(x_i)$ is the linear phase $\varphi = \langle p | x - \frac{q}{2} \rangle$.

1.3 The Heisenberg-Weyl Group

In this section we study the property of the Heisenberg-Weyl group and its action on the states. In particular we will show how to “create” Canonical Coherent States, starting from a Gaussian wave packet. We will see that these states satisfy the equation (1.2.2) and are related to the set $\mathfrak{G}_G$ of Gaussons. For this part we will follow mostly [Per86], [AAG00] and [CR12].
In the following we will treat only the 1-dimensional case, but everything can be done in the same way also for the n-dimensional case (component by component). The operators X and P acting on the Hilbert space $\mathcal{H}$, satisfy the Heisenberg commutation relation

$$[X, P] = \mathrm{i}\varepsilon I, \quad [X, I] = [P, I] = 0 \tag{1.3.1}$$

Instead of working with X and P, it is useful to define two new operators.

Definition 1.3.1. *The operators a and $a^\dagger$ defined as*

$$a^\dagger = \frac{X - \mathrm{i}P}{\sqrt{2\varepsilon}} \tag{1.3.2}$$

$$a = \frac{X + \mathrm{i}P}{\sqrt{2\varepsilon}} \tag{1.3.3}$$

are called creation and annihilation operators respectively.

Proposition 1.3.2. *The creation and annihilation operators satisfy*

$$[a, a^\dagger] = 1 \tag{1.3.4}$$

$$[a, I] = [a^\dagger, I] = 0 \tag{1.3.5}$$

Proof. Since it is a simple calculation using the properties of the commutator we prove only the first equality:

$$\begin{aligned}
[a, a^\dagger] &= \left[\frac{X + \mathrm{i}P}{2\sqrt{\varepsilon}}, \frac{X - \mathrm{i}P}{2\sqrt{\varepsilon}}\right] \\
&= \frac{1}{2\varepsilon}\left([X, X] + [P, P] + \mathrm{i}[P, X] - \mathrm{i}[X, P]\right) \\
&= \frac{1}{2\varepsilon}\left(\mathrm{i}[P, X] - \mathrm{i}[X, P]\right) \\
&= \frac{1}{2\varepsilon}\left(-2\mathrm{i}[X, P]\right) = \frac{-2\mathrm{i}^2\varepsilon}{2\varepsilon} I = I
\end{aligned}$$

□

We introduce three new operators

$$e_1 = \frac{\mathrm{i}P}{\sqrt{\varepsilon}}, \quad e_2 = \frac{\mathrm{i}X}{\sqrt{\varepsilon}}, \quad e_3 = \mathrm{i}I$$

that will generate the Lie algebra of the operators and we give the following definition.

Definition 1.3.3. *The Heisenberg-Weyl algebra $\mathcal{HW}$ is a real, three dimensional, Lie algebra, given by the commutation relations*

$$[e_1, e_2] = e_3, \quad [e_1, e_3] = [e_2, e_3] = 0$$

The elements of $\mathcal{HW}$ are written as a linear combination of the generators:

$$x = x(s; x_1, x_2) = x_1 e_1 + x_2 e_2 + s e_3 \tag{1.3.6}$$

where s, x_1 and x_2 are three real numbers and if we substitute

$$x_1 = -\frac{q}{\sqrt{\varepsilon}}, \quad x_2 = \frac{p}{\sqrt{\varepsilon}}$$

we can write the element of the algebra in terms of the operators X and P and of the point (q, p) in the following way

$$x(s; q, p) = \mathrm{i}sI + \frac{\mathrm{i}}{\varepsilon}(pX - qP) \tag{1.3.7}$$

There is another way to express the generic element of the Lie algebra as a function of the creation and annilhation operators by putting

$$x(s;\alpha) = \mathrm{i}sI + (\alpha a^\dagger - \bar{\alpha}a) \tag{1.3.8}$$

where

$$\alpha = \frac{q+\mathrm{i}p}{\sqrt{2\varepsilon}} = \frac{-x_1+\mathrm{i}x_2}{\sqrt{2}}, \quad \bar{\alpha} = \frac{q-\mathrm{i}p}{\sqrt{2\varepsilon}}$$

This last expression will be particularly useful in what will follow. Since we are working with a Lie algebra we have to define also the commutator of two elements: if $x = x(s; x_1, x_2)$ and $y = y(t; y_1, y_2)$ their commutator will be

$$[x, y] = (x_1y_2 - x_2y_1)e_3 = B(x, y)e_3$$

where $B(x, y)$ is the symplectic form on the (x_1, x_2)-plane.
To construct the corresponding Lie group from its algebra, one must use exponentiation: starting from expression (1.3.8) we have

$$\exp(x) = \exp(\mathrm{i}sI)\exp(\alpha a^\dagger - \bar{\alpha}a) = \exp(\mathrm{i}sI)D(\alpha) \tag{1.3.9}$$

where

$$D(\alpha) = \exp(\alpha a^\dagger - \bar{\alpha}a) \tag{1.3.10}$$

Note that we can rewrite in another form $D(\alpha)$ using the operators X and P and the point (q, p):

$$D(\alpha) = \exp\frac{\mathrm{i}}{\varepsilon}(pX - qP) \tag{1.3.11}$$

where we use (with an abuse of notation) the same symbol $D(\alpha)$ for the coordinates (q, p) and its complexification α. Now the problem is to find the multiplication law of the group. We start using the following identity (Baker-Campbell-Hausdorff)

$$\exp A \exp B = \exp\left(\frac{1}{2}[A, B]\right)\exp(A + B) \tag{1.3.12}$$

when $[A, [A, B]] = [B, [A, B]] = 0$.

Lemma 1.3.4. *We have*

$$D(\alpha)D(\beta) = \exp(\mathrm{i}Im\,(\alpha\bar{\beta}))D(\alpha + \beta) \tag{1.3.13}$$

Proof. Putting $A = \alpha a^\dagger - \bar{\alpha}a$ and $B = \beta a^\dagger - \bar{\beta}a$, we get

$$A + B = (\alpha + \beta)a^\dagger - (\bar{\alpha} + \bar{\beta})a$$

and so

$$\exp(A+B) = D(\alpha+\beta)$$

It remains only to compute $\exp(\frac{1}{2}[A,B])$:

$$\frac{1}{2}[A,B] = \frac{1}{2}[\alpha a^\dagger - \bar{\alpha}a, \beta a^\dagger - \bar{\beta}a] = \frac{1}{2}(\alpha\bar{\beta} - \bar{\alpha}\beta) = \mathrm{i}\,\mathrm{Im}(\alpha\bar{\beta})$$

that means

$$\exp\left(\frac{1}{2}[A,B]\right) = \exp(\mathrm{i}\,\mathrm{Im}(\alpha\bar{\beta}))$$

as required. □

We can write down explicitly the operator $D(\alpha)$ in terms of $\alpha, a, a^\dagger$ or using $(q,p), X, P$.

Lemma 1.3.5. *We have*

$$D(\alpha) = \exp\left(-\frac{|\alpha|^2}{2}\right)\exp\left(\alpha a^\dagger\right)\exp\left(-\bar{\alpha}a\right) = \exp\left(-\frac{\mathrm{i}}{\varepsilon}\frac{pq}{2}\right)\exp\left(\frac{\mathrm{i}}{\varepsilon}pX\right)\exp\left(-\frac{\mathrm{i}}{\varepsilon}qP\right) \quad (1.3.14)$$

Proof. Starting again from Weyl's identity

$$\exp(A+B) = \exp\left(-\frac{1}{2}[A,B]\right)\exp A \exp B \quad (1.3.15)$$

one has, recalling that $[\alpha a^\dagger, -\bar{\alpha}a] = -|\alpha|^2[a^\dagger, a] = |\alpha|^2 I$

$$D(\alpha) = \exp\left(\alpha a^\dagger - \bar{\alpha}a\right) = \exp\left(-\frac{|\alpha|^2}{2}\right)\exp\left(\alpha a^\dagger\right)\exp\left(-\bar{\alpha}a\right)$$

and the first equality is proven. Moreover we have, starting from (1.3.11) and using again (1.3.15) with $A = \frac{\mathrm{i}}{\varepsilon}pX$ and $B = -\frac{\mathrm{i}}{\varepsilon}qP$, noticing that

$$\frac{1}{2}[A,B] = -\frac{\mathrm{i}}{\varepsilon}\frac{pq}{2}$$

we get

$$\exp\left(\frac{\mathrm{i}}{\varepsilon}(pX - qP)\right) = \exp\left(-\frac{\mathrm{i}}{\varepsilon}\frac{pq}{2}\right)\exp\left(\frac{\mathrm{i}}{\varepsilon}pX\right)\exp\left(-\frac{\mathrm{i}}{\varepsilon}qP\right)$$

and the proof is completed. □

We want to understand how these operators act on a state of $\mathcal{H}$. To do this the following lemma is very useful.

Lemma 1.3.6.

$$e^{\frac{\mathrm{i}}{\varepsilon}pX}\psi(x) = e^{\frac{\mathrm{i}}{\varepsilon}px}\psi(x) \quad (1.3.16)$$

$$e^{-\frac{\mathrm{i}}{\varepsilon}qP}\psi(x) = \psi(x-q) \quad (1.3.17)$$

Proof. To prove the statements we use Taylor expansion of the exponential of the operator:

$$e^{\frac{\mathrm{i}}{\varepsilon}pX}\psi(x) = \sum_{n=0}^{\infty}\frac{1}{n!}p^n\left(\frac{\mathrm{i}}{\varepsilon}\right)^n x^n\psi(x) = \psi(x)\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\mathrm{i}}{\varepsilon}px\right)^n = e^{\frac{\mathrm{i}}{\varepsilon}px}\psi(x)$$

The second equality is obtained using the previous equality for the multiplication operator, but using the Fourier transform to have the $\{P\}$ representation for the wave function. In this case the P operator is again the multiplication operator by p, so, using the previous result, we have

$$e^{-\frac{\mathrm{i}}{\varepsilon}qP}\widehat{\psi}(p) = \sum_{n=0}^{\infty}\frac{1}{n!}(-q)^n\left(\frac{\mathrm{i}}{\varepsilon}\right)^n p^n\widehat{\psi}(p) = \widehat{\psi}(p)\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{\mathrm{i}}{\varepsilon}qp\right)^n = e^{-\frac{\mathrm{i}}{\varepsilon}qp}\widehat{\psi}(p)$$

and the last expression is exactly the Fourier transorm of the wave function $\psi(x-q)$, i.e. we have

$$e^{-\frac{\mathrm{i}}{\varepsilon}qP}\psi(x) = \psi(x-q)$$

□

We recollect everything in the following proposition.

Proposition 1.3.7. *In coordinates representation the action of the operator $D(\alpha)$ is given by*

$$D(\alpha)\psi(x) = \exp\left(\frac{\mathrm{i}}{\varepsilon}p\left(x-\frac{q}{2}\right)\right)\psi(x-q) \tag{1.3.18}$$

Proof. Follows immediately from the previous lemma. □

Remark 1.3.8 Suppose $x \in \mathbb{R}$ and to have as initial state

$$\psi(x) = \left(\frac{1}{\pi\varepsilon}\right)^{1/4} e^{-\frac{x^2}{2\varepsilon}}$$

then $D(\alpha)\psi(x)$ has the following form

$$D(\alpha)\psi(x) = \left(\frac{1}{\pi\varepsilon}\right)^{1/4} e^{-\frac{(x-q)^2}{2\varepsilon}} e^{\frac{\mathrm{i}}{\varepsilon}\langle p, x-\frac{q}{2}\rangle} = \eta^{U,V}_{(q,p)}(x)$$

as in (1.2.3) with $V=0$ and $U=\frac{1}{2\varepsilon}$. Now it is clear that the right constant $k \in \mathbb{R}$ that appears in Remark 1.1.3 is $pq/2$.

The operator-valued map $\alpha \mapsto D(\alpha) = \exp(\alpha a^\dagger - \bar{\alpha}a)$ is a unitary representation, up to a phase factor, of the group of translations of the complex plane. Starting from (1.3.13) and observing that

$$[A, B] = \mathrm{i}\mathrm{Im}\,(\alpha\bar{\beta}) = -2\mathrm{i}\alpha \wedge \beta$$

it is easy to verify the unitarity of the operator $D(\alpha)$:

$$D(\alpha)D(-\alpha) = e^{-\mathrm{i}\alpha\wedge\alpha}D(\alpha-\alpha) = I$$

and so $D(-\alpha) = \exp(\bar{\alpha}a - \alpha a^{\dagger}) = D(\alpha)^{\dagger} = D(\alpha)^{-1}$. We can extend the relation (1.3.13): considering $\alpha_1, \dots, \alpha_n$ we have

$$D(\alpha_n)\cdot \ldots \cdot D(\alpha_1) = e^{\mathrm{i}\delta}D(\alpha_1 + \ldots + \alpha_n)$$

where the phase $\delta = -\sum_{k<j}\alpha_k \wedge \alpha_j$ has a (symplectic) topological meaning: it is equal to the oriented area of the poligon width edges $\alpha_1, \alpha_1+\alpha_2, \dots, \alpha_1+\ldots+\alpha_n$. In canonical coordinates $z_j = (q_j + p_j)/\sqrt{2}$ and we have

$$\delta = \sum_{j<k}\frac{1}{2}\left(q_j p_k - q_k p_j\right) \tag{1.3.19}$$

1.3.1 The set of canonical Coherent States

Now we give the general definition of the Heisenberg-Weyl group $G_{\mathcal{HW}}$.

Definition 1.3.9. *The Heisenberg Weyl group $G_{\mathcal{HW}}$ is the set of elements g of the form*

$$g = (s,q,p), \;\; s\in\mathbb{R}, \;\; (q,p)\in\mathbb{R}^{2n}$$

with the multiplication law

$$g_1g_2 = (s_1+s_2+\xi((q_1,p_1),(q_2,p_2)), q_1+q_2, p_1+p_2)$$

where ξ is the multiplier function

$$\xi((q_1,p_1),(q_2,p_2)) = \frac{1}{2}(\langle p_1,q_2\rangle - \langle p_2,q_1\rangle)$$

Remark 1.3.10 We can rewrite the previous relation in the coordinates (q,p). Then every element $g\in G_{\mathcal{HW}}$ will be given by

$$g = (s,\alpha), \;\; s\in\mathbb{R}, \;\; \alpha\in\mathbb{C}$$

with multiplication law

$$g_1g_2 = (s_1+s_2+\xi(\alpha,\beta), \alpha+\beta)$$

with $\xi(\alpha,\beta) = \mathrm{Im}(\alpha\bar{\beta})$. Note that the function ξ coincides with δ in (1.3.19).

Now we call Θ the phase subgroup of $G_{\mathcal{HW}}$, that means the set of elements of the form $g = (s, 0, 0)$ with $s \in \mathbb{R}$. Then the quotient group $G_{\mathcal{HW}}/\Theta$ can be identified with $\mathbb{R}^{2n}$ and parametrized by (q, p) (or equivalently using $\alpha \in \mathbb{C}^n$). With this parametrization $G_{\mathcal{HW}}/\Theta$ carries the invariant measure

$$d\nu(q,p) = \frac{dqdp}{2\pi}$$

and the function

$$\begin{aligned} \sigma : G_{\mathcal{HW}}/\Theta &\to G_{\mathcal{HW}} \\ \sigma(q,p) &= (0,q,p) \end{aligned}$$

defines a section in $G_{\mathcal{HW}}$, and it can be viewed as a fiber bundle over $G_{\mathcal{HW}}/\Theta$, with fibers isomorphic to θ. In this way we can define the set of canonical Coherent States.

Definition 1.3.11 ([AAG00])**.** *The set*

$$\mathfrak{S}_{CCS} = \{\eta_{(q,p)} = D(\alpha)\eta \mid (q,p) \in G_{\mathcal{HW}}/\Theta\}$$

where $D(\alpha)\eta = e^{\frac{i}{\varepsilon}\langle p, x - \frac{q}{2}\rangle}\eta(x-q)$ *and*

$$\eta(x) = \left(\frac{1}{\pi\varepsilon}\right)^{n/4} \prod_{i=1}^{n} e^{-\frac{x_i^2}{2\varepsilon}}$$

is a Gaussian Wave Packet, is called the set of Canonical Coherent States.

Remark 1.3.12 It easy to see that the set of Canonical Coherent States is a subset of the set of Gaussons: $\mathfrak{S}_{CCS} \subset \mathfrak{S}_G$. More precisely one has that

$$\mathfrak{S}_{CCS} = \left\{ \eta^{U,V}_{(q,p)} \in \mathfrak{S}_G \;\middle|\; U = \frac{1}{\varepsilon} I,\, V = 0 \right\}$$

Proposition 1.3.13. *Every Canonical Coherent State* $\eta_{(q,p)} \in \mathfrak{S}_{CCS}$ *satisfies (1.2.2).*

Proof. It is an easy computation: the phase function for a Canonical Coherent State is $\varphi_{(q,p)}(x) = p \cdot (x - \frac{q}{2})$ and its i-th partial derivative $\partial_{x_i}\varphi_{(q,p)}(x) = p_i$. Then (using the notations in (1.2.2)) one has

$$\left[\left(\partial_{x_i}\varphi_{(q,p)}\right)^2 * \mathcal{G}\right](q) = p_i^2 C(\varepsilon)\int_{\mathbb{R}^n}\prod_{i=1}^n e^{-\frac{(x_i-q_i)^2}{2\varepsilon}}dx_1\dots dx_n = p_i^2$$

$$\left[\partial_{x_i}\varphi_{(q,p)} * \mathcal{G}\right]^2(q) = \left[C(\varepsilon)\int_{\mathbb{R}^n} p_i\prod_{i=1}^n e^{-\frac{(x_i-q_i)^2}{2\varepsilon}}dx_1\dots dx_n\right]^2 = p_i^2$$

as required. □

1.4 Coherent States on the torus

In this section we want to underline the fact that it is possible to speak of coherent states on the torus $\mathbb{T}^n$. For example, if we want a Gaussian coherent state $\psi_{(q,p)}(x)$ with $x \in \mathbb{T}$ and $(q,p) = (0,0)$, we have

$$\psi_{(0,0)}(x) = \left(\frac{\pi}{\varepsilon}\right)^{1/4}\sum_n e^{-\frac{n^2}{2}\varepsilon}e^{inx}$$

because it is simply the coherent state on $\mathbb{R}$ where we have applied the Poisson Summation Formula.

Proposition 1.4.1. *Let g be the Gaussian on $\mathbb{R}$. Then*

$$\sum_{k=-\infty}^{+\infty} g(x+2\pi k) = \frac{1}{2\pi}\sum_{n=-\infty}^{+\infty}\widehat{g}(n)e^{inx}$$

where

$$\widehat{g}(n) = \sqrt{2\pi\varepsilon}\, e^{-\frac{n^2}{2}\varepsilon}$$

is the Fourier Transform of the Gaussian.

Proof. Let

$$h(x) = \sum_{k=-\infty}^{+\infty} g(x+2\pi k)$$

then h is 2π-periodic and its Fourier coefficients are

$$\widehat{h}_n = \frac{1}{2\pi}\int_0^{2\pi} h(x)e^{-\mathrm{i}nx}dx = \frac{1}{2\pi}\sum_{k=-\infty}^{+\infty}\int_0^{2\pi} g(x+2\pi k)e^{-\mathrm{i}nx}dx$$

$$= \frac{1}{2\pi}\sum_{k=-\infty}^{+\infty}\int_{2\pi k}^{2\pi(k+1)} g(x)e^{-\mathrm{i}nx}dx = \frac{1}{2\pi}\int_{-\infty}^{+\infty} g(x)e^{-\mathrm{i}nx}dx = \frac{1}{2\pi}\widehat{g}(n)$$

and this concludes the proof. □

It is also possible to consider a Gaussian coherent state $\varphi_{\alpha,Z}(x)$ with $\alpha = (q,p) \in \mathbb{R}^2$, $Z \in M_{n\times n}(\mathbb{C})$ with $\operatorname{Im} Z > 0$ and its periodisation $\varphi^{(\theta)}_{\alpha,Z} = \Sigma^{(\theta)}_N \varphi_{\alpha,Z}$. More precisely $\Sigma^{(\theta)}_N$ is the periodisation operator acting on the states in the following way

$$\Sigma^{(\theta)}_N = \sum_{z\in\mathbb{Z}^2} (-1)^{Nz_1z_2} e^{\mathrm{i}(\theta_1 z_1 - \theta_2 z_2)} \widehat{T}(z) \tag{1.4.1}$$

where

$$\widehat{T}(z)\psi(x) = e^{-\mathrm{i}z_1z_2/2\varepsilon} e^{\mathrm{i}xz_2/\varepsilon} \psi(x - z_1) \tag{1.4.2}$$

and we suppose that $N = \frac{1}{2\pi\varepsilon}$ (or equivalently the Planck's constant can be obtained as $\varepsilon = \frac{1}{2\pi N}$). In this case the state $\varphi^{(\theta)}_{\alpha,Z}$ is equal to

$$\varphi^{(\theta)}_{\alpha,Z} = \sum_{n_1,n_2\in\mathbb{Z}} (-1)^{Nn_1n_2} e^{\mathrm{i}(\theta_1 n_1 - \theta_2 n_2) + \frac{\mathrm{i}}{2\varepsilon}\sigma(n,z)} D(n+z)\varphi_{0,Z} \tag{1.4.3}$$

(see [CR12] for proofs), where σ is the symplectic form

$$\sigma((a,b),(c,d)) = ad - bc$$

and D is as in (1.3.18).

1.5 The symplectic group and the Siegel upper half space

Here we want to recall some results on the linear symplectic group $\mathrm{Sp}(n,\mathbb{R})$ that will be useful in the following sections. We define

$$\mathcal{J} := \begin{pmatrix} \mathbb{O} & -\mathbb{I} \\ \mathbb{I} & \mathbb{O} \end{pmatrix} \tag{1.5.1}$$

Clearly one has the following equalities

$$\mathcal{J}^2 = -\mathbb{I}$$
$$\mathcal{J}^T = -\mathcal{J} = \mathcal{J}^{-1}$$

Definition 1.5.1. *A matrix $\mathcal{A} \in M_{2n\times 2n}(\mathbb{R})$ will be called a symplectic matrix if*

$$\mathcal{A}^T \mathcal{J} \mathcal{A} = \mathcal{J} \tag{1.5.2}$$

and we will write $\mathcal{A} \in Sp(n,\mathbb{R})$.

Moreover we define the symplectic Lie algebra in the following way.

Definition 1.5.2. *The symplectic Lie algebra $\mathfrak{sp}(n,\mathbb{R})$ is the set of matrix $A \in M_{2n\times 2n}(\mathbb{R})$ such that $e^{At} \in Sp(n,\mathbb{R})$ for all $t \in \mathbb{R}$.*

First we recall two results on the polar decomposition of a matrix.

Proposition 1.5.3. *(i) If $\mathcal{A} \in GL(2n, \mathbb{R})$ then*

$$\mathcal{A} = \mathcal{U}\mathcal{P} \tag{1.5.3}$$

where $\mathcal{U} \in \mathcal{O}(2n)$ and $\mathcal{P}$ is positive definite.

(ii) If $\mathcal{A} \in Sp(n, \mathbb{R})$ then

$$\mathcal{A} = \mathcal{U}\mathcal{P} \tag{1.5.4}$$

with $\mathcal{U}$ and $\mathcal{P}$ as before and $\mathcal{U}, \mathcal{P} \in Sp(n, \mathbb{R})$.

Proof. (i) If $\mathcal{A} = \mathcal{U}\mathcal{P}$ with $\mathcal{U} \in \mathcal{O}(2n)$ and $\mathcal{P} > 0$ then

$$\mathcal{A}^T\mathcal{A} = \mathcal{P}^T\mathcal{U}^T\mathcal{U}\mathcal{P} = \mathcal{P}^T\mathcal{P} = \mathcal{P}^2$$

and so we must have $P = (\mathcal{A}^T\mathcal{A})^{1/2}$. Note that since $\mathcal{A}^T\mathcal{A}$ is positive definite then $\mathcal{P}$ is. So we must have $\mathcal{U} = \mathcal{A}\mathcal{P}^{-1}$ and

$$(\mathcal{A}\mathcal{P}^{-1})^T\mathcal{A}\mathcal{P}^{-1} = \mathcal{P}^{-T}\mathcal{A}^T\mathcal{A}\mathcal{P}^{-1} = \mathcal{P}^{-T}\mathcal{P}^T\mathcal{P}\mathcal{P}^{-1} = \mathbb{I}$$

and we get $\mathcal{U} \in \mathcal{O}(2n)$ as required.

(ii) First note that if $\mathcal{A}$ is symplectic then

$$\mathcal{A}^{-T} = \mathcal{J}\mathcal{A}\mathcal{J}^{-1}$$

and since $\mathcal{A}$ admits a unique polar decomposition by (i) we get

$$\mathcal{U}^{-T}\mathcal{P}^{-T} = \mathcal{J}\mathcal{U}\mathcal{P}\mathcal{J}^{-1} = (\mathcal{J}\mathcal{U}\mathcal{J}^{-1})(\mathcal{J}\mathcal{P}\mathcal{J}^{-1})$$

Since $\mathcal{J}\mathcal{U}\mathcal{J}^{-1}$ is orthogonal then we have $\mathcal{J}\mathcal{U}\mathcal{J}^{-1} = \mathcal{U}^{-T}$ and so $\mathcal{U}$ is symplectic. Moreover $\mathcal{J}\mathcal{P}\mathcal{J}^{-1}$ is positive definite and so $\mathcal{J}\mathcal{P}\mathcal{J}^{-1} = \mathcal{P}^{-T}$ that means $\mathcal{P} \in \mathrm{Sp}(n, \mathbb{R})$.

$\square$

Proposition 1.5.4. *$Sp(n, \mathbb{R}) \cap \mathcal{O}(2n)$ is a maximal compact subgroup of $Sp(n, \mathbb{R})$.*

Proof. Let K be a subgroup of $\mathrm{Sp}(n, \mathbb{R})$ containing $\mathrm{Sp}(n, \mathbb{R}) \cap \mathcal{O}(2n)$, we choose $\mathcal{A} \in K$ and we show that $\mathcal{A} \in \mathrm{Sp}(n, \mathbb{R}) \cap \mathcal{O}(2n)$. Using the previous proposition we have $\mathcal{A} = \mathcal{U}\mathcal{P}$ and since $\mathcal{U} \in \mathcal{O}(2n)$ then $\mathcal{U} \in K$. From this fact we must have also $\mathcal{P} = \mathcal{U}^{-1}\mathcal{A} \in K$. $\mathcal{P}$ is positive definite and $\det \mathcal{P} = 1$ (from the fact that $\mathcal{P}^T\mathcal{J}\mathcal{P} = \mathcal{J}$), that implies either $\mathcal{P} = \mathbb{I}$ or $\mathcal{P}$ has some eigenvalue greater than 1. If $\mathcal{P} = \mathbb{I}$ then $\mathcal{A} = \mathcal{U} \in \mathcal{O}(2n)$; otherwise we must have $\mathcal{P}^j \in K$ for all j but $\|\mathcal{P}^j\| \to \infty$ implying that K is not compact. $\square$

Proposition 1.5.5. *$Sp(n, \mathbb{R})$ is connected and $\mathbb{Z}$ is its fundamental group.*

Proof. First note that if $\mathcal{P} \in \mathrm{Sp}(n, \mathbb{R})$ then $\mathcal{P}$ is positive definite if and only if $\mathcal{P} = e^{\mathfrak{B}}$ where $\mathfrak{B} \in \mathfrak{sp}(n, \mathbb{R})$ and $\mathfrak{B} = \mathfrak{B}^T$. Moreover if we identify $\mathbb{R}^{2n}$ with $\mathbb{C}^n$ using $(q, p) \mapsto q + \mathrm{i}p$, then $\mathrm{Sp}(n, \mathbb{R}) \cap O(2n) = U(n)$. So $\mathrm{Sp}(n, \mathbb{R})$ is topologically equivalent to the product $U(n) \times \{\mathfrak{B} \in \mathfrak{sp}(n, \mathbb{R}) \,|\, \mathfrak{B} = \mathfrak{B}^T\}$ and the proposition follows from the well known properties of $U(n)$. □

Proposition 1.5.6. *The subsets of $GL(2n, \mathbb{R})$*

$$N = \left\{ \begin{pmatrix} \mathbb{I} & F \\ \mathbb{O} & \mathbb{I} \end{pmatrix} : F = F^T \right\}, \quad \bar{N} = \left\{ \begin{pmatrix} \mathbb{I} & \mathbb{O} \\ G & \mathbb{I} \end{pmatrix} : G = G^T \right\}$$

$$D = \left\{ \begin{pmatrix} E & \mathbb{O} \\ \mathbb{O} & E^{-T} \end{pmatrix} : E \in GL(n, \mathbb{R}) \right\}$$

are subgroups of $Sp(n, \mathbb{R})$. Moreover

$$\bar{N}DN = \left\{ \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp(n, \mathbb{R}) : \det A \neq 0 \right\}$$

Proof. The first part of the proposition is very easy to prove. Suppose now that we have three matrices (one for every subgroup) and we multiply them. We obtain:

$$\begin{pmatrix} \mathbb{I} & \mathbb{O} \\ G & \mathbb{I} \end{pmatrix} \begin{pmatrix} E & \mathbb{O} \\ \mathbb{O} & E^{-T} \end{pmatrix} \begin{pmatrix} \mathbb{I} & F \\ \mathbb{O} & \mathbb{I} \end{pmatrix} = \begin{pmatrix} E & EF \\ GE & GEF + E^{-T} \end{pmatrix} \tag{1.5.5}$$

where the last matrix is symplectic and $\det E \neq 0$ since $E \in \mathrm{GL}(n, \mathbb{R})$. To complete the proof we will show that every symplectic matrix $\mathcal{S} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ with $\det A \neq 0$ can be written as the product of three matrices as in the statement of the proposition. Consider again (1.5.5). One takes $E = A$, $F = A^{-1}B$ and $G = CA^{-1}$ and we have to prove that $F = F^T$, $G = G^T$ and $D = GEF + E^{-T}$. Since $\mathcal{S}$ is symplectic we have $\mathcal{S}^T \mathcal{J} \mathcal{S} = \mathcal{J}$ that implies $A^T C = C^T A$, $AB^T = BA^T$ and $A^T D - C^T B = \mathbb{I}$. Using the first two relations we have

$$\begin{cases} A^T C = C^T A \Rightarrow E^T G E = E^T G^T E \Rightarrow G = G^T \\ AB^T = BA^T \Rightarrow EF^T E^T = EFE^T \Rightarrow F = F^T \end{cases}$$

It remains to show that $D = GEF + E^{-T}$ but $D = A^{-T} C^T B + A^{-T} = E^{-T} E^T G^T EF + E^{-T} = GEF + E^{-T}$. □

Theorem 1.5.7. *$Sp(n, \mathbb{R})$ is generated by $D \cup N \cup \{\mathcal{J}\}$ or by $D \cup \bar{N} \cup \{\mathcal{J}\}$.*

Proof. It is easy to verify that $\mathcal{J} \bar{N} \mathcal{J}^{-1} = N$ and $\mathcal{J}^{-1} \in \mathcal{J} D$. Define G as the subgroup generated by $D \cup N \cup \{\mathcal{J}\}$ (or equivalently by $D \cup \bar{N} \cup \{\mathcal{J}\}$). It will contain $\bar{N}DN$ and, since $\bar{N}DN$ is an open neighborhood of the identity, G is open and also closed (its complement is an union of cosets and so open). This implies, since $\mathrm{Sp}(n,\mathbb{R})$ is connected, that $G = \mathrm{Sp}(n,\mathbb{R})$. $\square$

The last theorem will be useful in the next sections: it tells us that every symplectic matrix can be written as the product

$$\mathcal{S} = \begin{pmatrix} A & \mathbb{O} \\ \mathbb{O} & A^{-T} \end{pmatrix} \begin{pmatrix} \mathbb{I} & B \\ \mathbb{O} & \mathbb{I} \end{pmatrix} \mathcal{J}$$

or as

$$\mathcal{S} = \begin{pmatrix} A & \mathbb{O} \\ \mathbb{O} & A^{-T} \end{pmatrix} \begin{pmatrix} \mathbb{I} & \mathbb{O} \\ B & \mathbb{I} \end{pmatrix} \mathcal{J} \tag{1.5.6}$$

If we choose a coherent state with phase

$$\langle p, x-q\rangle + \frac{1}{2}\langle Z(x-q), x-q\rangle$$

then we can associate to it the Lagrangian submanifold

$$\{(x, p + Z(x-q)) : x \in \mathbb{R}^n\} = \{(q+x, p+Zx) : x \in \mathbb{R}^n\}$$

that is a submanifold of $T_{(q,p)}(T^*M)$. If Z is complex we have to "complexify" the tangent space. Let (V,ω) be a symplectic vector space over $\mathbb{R}$ of dimension $2n$ and denote with $V^{\mathbb{C}}$ its complexification. A subspace $L \subset V$, or $L \subset V^{\mathbb{C}}$, is called Lagrangian if $\dim L = n$, or $\dim_{\mathbb{C}} L = n$ respectively, and

$$\omega(z_1, z_2) = 0 \text{ for all } z_1, z_2 \in L$$

Definition 1.5.8. *The set of all Lagrangian planes in V is called Lagrangian Grassmannian and denoted with $\Lambda(V)$. Similarly $\Lambda(V^{\mathbb{C}})$ is the Lagrangian Grassmannian of the complexification. A Lagrangian plane $L \in \Lambda(V^{\mathbb{C}})$ is called positive if*

$$\mathrm{i}\omega(\bar{z}, z) \geq 0 \text{ for all } z \in L$$

and totally real if

$$\mathrm{i}\omega(\bar{z}, z) = 0 \text{ for all } z \in L$$

The set of all positive Lagrangian planes in $V^{\mathbb{C}}$ will be denoted by $\Lambda^+(V^{\mathbb{C}})$.

Definition 1.5.9. *Let L_0 be a totally real Lagrangian plane in $V^{\mathbb{C}}$. We denote with*

$$\Lambda^+_{L_0}(V^{\mathbb{C}}) := \left\{L \in \Lambda^+(V^{\mathbb{C}}) : L \cap L_0\right\}$$

the space of all the Lagrangian planes transversal to L_0.

Lemma 1.5.10. *$\Lambda^+_{L_0}(V^{\mathbb{C}})$ is isomorphic to the space of all symmetric $n \times n$ matrices with positive imaginary part.*

Definition 1.5.11. *The set of symmetric $n \times n$ matrices Z with positive imaginary part is called Siegel upper half space Σ_n.*

Let $\mathcal{S} \in \mathrm{Sp}(n, \mathbb{R})$ be a $2n \times 2n$ symplectic matrix of the form

$$\mathcal{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

The linear symplectic group $\mathrm{Sp}(n, \mathbb{R})$ acts on the set of Lagrangian planes: infact there is a bijection between the set of complex Lagrangian planes and the set of complex symmetric matrices. A complex Lagrangian plane is the set $L_Z = \{(x, Zx),\ x \in \mathbb{C}^n\}$. Let Z a $n \times n$ complex matrix with $\operatorname{Im} Z > 0$. We look for a matrix $\mathcal{S}_* Z$ such that

$$\mathcal{S} L_Z = L_{\mathcal{S}_* Z} \tag{1.5.7}$$

where $L_Z = \{(x, Zx),\ x \in \mathbb{C}^n\}$ and $L_{\mathcal{S}_* Z} = \{(x, \mathcal{S}_* Zx),\ x \in \mathbb{C}^n\}$, then the equation (1.5.7) reads

$$\begin{aligned} (S_{11} + S_{12} Z)x &= y \\ (S_{21} + S_{22} Z)x &= \mathcal{S}_* Z y \end{aligned}$$

and inserting the first equation in the second, one gets

$$\mathcal{S}_* Z = (S_{21} + S_{22} Z)(S_{11} + S_{12} Z)^{-1} \tag{1.5.8}$$

Theorem 1.5.12. *(i) If $\mathcal{T}, \mathcal{S} \in Sp(n, \mathbb{R})$ and $Z \in \Sigma_n$ then $\mathcal{T}_* \mathcal{S}_* Z = (\mathcal{T}\mathcal{S})_* Z$.*

(ii) If $Z \in \Sigma_n$ and $\mathcal{S} \in Sp\,(n, \mathbb{R})$ then $\mathcal{S}_* Z \in \Sigma_n$;

(iii) for any $Z_1, Z_2 \in \Sigma_n$, there exists an $\mathcal{S} \in Sp\,(n, \mathbb{R})$ with $\mathcal{S}_* Z_1 = Z_2$.

Proof. It is easy to prove (i). To prove (ii) we have to observe that

$$\begin{pmatrix} A & \mathbb{O} \\ \mathbb{O} & A^{-T} \end{pmatrix}_* Z = AZA^T, \quad \begin{pmatrix} \mathbb{I} & B \\ \mathbb{O} & \mathbb{I} \end{pmatrix}_* Z = Z + B, \quad \mathcal{J}_* Z = -Z^{-1}$$

and, since A is real, B is real and symmetric and $Z \in \Sigma_n$, then AZA^T and $Z + B$ are in Σ_n. Moreover $-Z^{-1}$ is symmetric and

$$\operatorname{Im}(-\overline{v} Z^{-1} v) = \operatorname{Im}(-w \overline{Zw}) = \operatorname{Im}(\overline{w} Z w) > 0$$

for all $v = Zw \neq 0$. Since we have prove the statement on the generators of $\mathrm{Sp}(n, \mathbb{R})$ we have the result.

$\square$

1.6 Propagation of Coherent States

We will follow mainly [CR97], [Rob98] and [Sch01]. In this section we want to understand the evolution of a coherent state in $\mathbb{R}^n$ centered at a point (q,p) of the phase space $\mathbb{R}^{2n}$. In the following we will consider the self adjoint operator

$$H = -\frac{\varepsilon^2}{2}\Delta + V(x) \tag{1.6.1}$$

where $x \in \mathbb{R}^n$, $V(x) \in C^\infty(\mathbb{R}^n)$ and H acts on $L^2(\mathbb{R}^n)$. Corresponding to this operator there is also its symbol

$$h(q,p) = \frac{\langle p, p\rangle}{2} + V(x) \tag{1.6.2}$$

that is the Hamiltonian function defined on $\mathbb{R}^{2n}$. Our aim will be to approximate the solution of the Cauchy problem

$$\begin{cases} \mathrm{i}\varepsilon\partial_t \phi(t,x) = H\phi(t,x) \\ \\ \phi(0,x) = \psi_{(q,p)}(x) = \left(\dfrac{1}{\pi\varepsilon}\right)^{n/4} e^{-\frac{|x-q|^2}{2\varepsilon}} e^{\frac{\mathrm{i}}{\varepsilon}\langle p, x-q\rangle} \end{cases} \tag{1.6.3}$$

so, from now on, $\phi(t,x) = e^{-\frac{\mathrm{i}}{\varepsilon}Ht}\psi_{(q,p)}(x)$ will represent the exact solution of the problem (1.6.3). Before proceeding in this direction, we need to understand how the error of an approximate solution propagates in time.

Lemma 1.6.1. *Let H be a self-adjoint operator and $\psi(t,x)$ and $\phi(t,x)$ such that*

$$\mathrm{i}\varepsilon\partial_t \psi(t,x) = H\psi(t,x) + R\psi(t,x)$$
$$\mathrm{i}\varepsilon\partial_t \phi(t,x) = H\phi(t,x)$$
$$\psi(0,x) - \phi(0,x) = \alpha^0(x)$$

Then for all $t \geq 0$ one has

$$\|\psi(t,\cdot) - \phi(t,\cdot)\|_{L^2} = O\Big(\|\alpha^0\|_{L^2} + \frac{t}{\varepsilon}\sup_{s\in[0,t]}\|R\psi(s,\cdot)\|_{L^2}\Big)$$

Proof. Once we define $e^{-\frac{\mathrm{i}}{\varepsilon}tH}\alpha(t,x) := \psi(t,x) - \phi(t,x)$, we get

$$\mathrm{i}\varepsilon\partial_t(\psi(t,x) - \phi(t,x)) = H(\psi(t,x) - \phi(t,x)) + R\psi(t,x)$$

and

$$
\begin{aligned}
e^{-\frac{\mathrm{i}}{\varepsilon}tH}(\mathrm{i}\varepsilon\partial_t\alpha(t,x)) + He^{-\frac{\mathrm{i}}{\varepsilon}tH}\alpha(t,x) &= He^{-\frac{\mathrm{i}}{\varepsilon}tH}\alpha(t,x) + R\psi(t,x) \\
\partial_t\alpha(t,x) &= \frac{1}{\mathrm{i}\varepsilon}e^{\frac{\mathrm{i}}{\varepsilon}tH}R\psi(t,x)
\end{aligned}
$$

From the last equality

$$
\alpha(t,x) = \alpha^0(x) + \frac{1}{\mathrm{i}\varepsilon}\int_0^t e^{\frac{\mathrm{i}}{\varepsilon}sH}R\psi(s,x)ds
$$

and easily applying the L^2 norm

$$
\|\alpha(t,\cdot)\|_{L^2} \le \|\alpha^0\|_{L^2} + \frac{t}{\varepsilon}\sup_{s\in[0,t]}\|R\psi(s,\cdot)\|_{L^2}
$$

we get the estimate of the Theorem. □

Before stating the main result of this part, we need one more proposition.

Proposition 1.6.2. *Consider the following Cauchy problem*

$$
\begin{cases}
-\dot{Z} = Z^2 + V''_{x,x}(q) \\
Z(0) = Z_0
\end{cases}
\tag{1.6.4}
$$

where $Z(t)$ is a $n\times n$ complex-valued matrix and $V''_{x,x}$ is the Hessian of the potential V. Let

$$
Z(t) = \mathcal{S}(t)_* Z_0 = (S_{21} + S_{22}Z_0)(S_{11} + S_{12}Z_0)^{-1}
\tag{1.6.5}
$$

where $\mathcal{S}(t)$ is the $2n\times 2n$ symplectic matrix solving the linearized equations

$$
\begin{cases}
\dot{\mathcal{S}} = \mathcal{J}H''\mathcal{S} = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ -V''_{x,x}(q(t)) & \mathbb{O} \end{pmatrix}\mathcal{S} \\
\mathcal{S}(0) = \mathbb{I}
\end{cases}
\tag{1.6.6}
$$

where H'' is the Hessian of the Hamiltonian $h(q,p) = \frac{1}{2}\langle p,p\rangle + V(x)$. Then $Z(t)$ is a solution of (1.6.4).

Proof. We start computing

$$
\begin{pmatrix} \dot{S}_{11} & \dot{S}_{12} \\ \dot{S}_{21} & \dot{S}_{22} \end{pmatrix} = \begin{pmatrix} S_{21} & S_{22} \\ -V''(q(t))S_{11} & -V''(q(t))S_{12} \end{pmatrix}
$$

Now

$$\begin{aligned}\dot{Z} &= (\dot{S}_{21} + \dot{S}_{22}Z_0)(S_{11} + S_{12}Z_0)^{-1} \\ &-(S_{21} + S_{22}Z_0)(S_{11} + S_{12}Z_0)^{-1}(\dot{S}_{11} + \dot{S}_{12}Z_0)(S_{11} + S_{12}Z_0)^{-1} \\ &= (\dot{S}_{21} + \dot{S}_{22}Z_0)(S_{11} + S_{12}Z_0)^{-1} - Z(\dot{S}_{11} + \dot{S}_{12}Z_0)(S_{11} + S_{12}Z_0)^{-1}\end{aligned}$$

and

$$\begin{aligned}\dot{S}_{11} + \dot{S}_{12}Z_0 &= S_{21} + S_{22}Z_0 \\ \dot{S}_{21} + \dot{S}_{22}Z_0 &= -V''(q(t))S_{11} - V''(q(t))S_{12}Z_0 = -V''(q(t))(S_{11} + S_{12}Z_0)\end{aligned}$$

Substituting into the equation for $\dot{Z}(t)$, we have

$$\dot{Z} = -V''(q(t)) - Z^2$$

that is exactly (1.6.4). Moreover $Z(0) = \mathbb{I}_* Z_0 = (\mathbb{I}Z_0)(\mathbb{I})^{-1} = Z_0$. □

The following Theorem tells us that we can approximate the solution of (1.6.3) using coherent states, but we have to make the initial state evolve using the classical Hamiltonian. With this approximation we make an error of order $\sqrt{\varepsilon}$. The statements are given in the articles of T. Paul in [Pau09], [Pau07b] and [Pau07a]. For a different proof see [Hag80]. Here we propose a different proof.

Theorem 1.6.3 (Paul [Pau07b])**.** *Let $V(x) \in C^3(\mathbb{R}^n)$ a function with bounded derivatives and $\phi(t,x) = e^{-\frac{\mathrm{i}}{\varepsilon}tH}\psi_{(q,p)}(x)$ be the solution of (1.6.3). Then there exist a generalized coherent state $\psi^{a,V}_{(q,p)}$ as in Definition (1.2.6), where $a = a(t), V = V(t)$ are given in (1.6.18) below, $(q,p) = (q(t),p(t))$ solve the classical system*

$$\begin{cases} \dot{q}(t) = \dfrac{\partial h}{\partial p}(q(t),p(t)) \\ q(0) = q \\ \dot{p}(t) = -\dfrac{\partial h}{\partial q}(q(t),p(t)) \\ p(0) = p \end{cases} \tag{1.6.7}$$

such that

$$\left\|\phi(t,\cdot) - e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)}\psi^{a(t)}_{(q(t),p(t))}(\cdot)\right\|_{L^2} \le C\varepsilon^{1/2} t \sup_{s\in[0,t]} |\operatorname{Im} Z(s)|_\infty^{-3/2} \tag{1.6.8}$$

where $Z(t)$ is a complex matrix $n \times n$, $|\cdot|_\infty$ is the matrix sup norm and the phase factor $\Theta(t)$ is given by

$$\Theta(t) = \int_0^t \Big[p(s)\dot{q}(s) - H(q(s),p(s))\Big] ds \tag{1.6.9}$$

Proof. In the following $\psi(t,x)$ will represent the approximate solution of (1.6.3). We will divide the proof in two steps:

(i) determine $a(t), V(t), (q(t), p(t)), \Theta(t)$;

(ii) compute and estimate the remainder $R\psi(t,x)$;

(i) We start rewriting the initial datum as

$$\begin{aligned}\psi_{(q,p)}(x) &= \left(\frac{1}{\pi\varepsilon}\right)^{n/4} e^{-\frac{(x-q)^2}{2\varepsilon}} e^{\frac{\mathrm{i}}{\varepsilon}\langle p, x-q\rangle} \\ &= \left(\frac{1}{\pi\varepsilon}\right)^{n/4} (\det \operatorname{Im} Z_0)^{1/4} e^{\frac{\mathrm{i}}{\varepsilon}[\langle p, x-q\rangle + \langle Z_0(x-q), x-q\rangle/2]}\end{aligned}$$

where we have chosen $Z_0 = \mathrm{i}\mathbb{I}$. Then we look for an approximate solution of the form

$$\psi(t,x) = \alpha(t) e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} e^{\frac{\mathrm{i}}{\varepsilon}[\langle p(t), x-q(t)\rangle + \langle Z(t)(x-q(t)), x-q(t)\rangle/2]}$$

under the condition that $\psi(0,x) = \psi_{(q,p)}(x)$. We insert $\psi(t,x)$ in the Schrödinger equation and we get:

$$\begin{aligned}(\mathrm{i}\varepsilon\dot{\alpha}/\alpha - \dot{\Theta} - \langle \dot{p}, x-q\rangle + \langle p, \dot{q}\rangle + \langle Z\dot{q}, (x-q)\rangle - \langle \dot{Z}(x-q), (x-q)\rangle/2)\psi = \\ = (-\mathrm{i}\varepsilon \operatorname{tr} Z/2 + (p + Z(x-q))^2/2 + V(x))\psi\end{aligned}$$

Now we develop the potential $V(x)$ in powers of $x-q$ and, up to second order, we get

$$\mathrm{i}\varepsilon\frac{\dot{\alpha}}{\alpha} - \dot{\Theta} - \langle p, \dot{q}\rangle = -\frac{\mathrm{i}\varepsilon}{2}\operatorname{tr} Z + \frac{|p|^2}{2} + V(q) \tag{1.6.10}$$

$$-\dot{p} + Z\dot{q} = Zp + V'_x(q) \tag{1.6.11}$$

$$-\dot{Z} = Z^2 + V''_{x,x}(q) \tag{1.6.12}$$

From (1.6.11) we get the following Cauchy problem

$$\begin{cases} \dot{p} = -V'_x(q) \\ p(0) = p \\ \dot{q} = p \\ q(0) = q \end{cases} \tag{1.6.13}$$

and taking $q(t)$ and $p(t)$ as the solutions of the Hamilton equations relative to

$$h(q,p) = \frac{|p|^2}{2} + V(q)$$

then the equation (1.6.11) is automatically satisfied.
Equation (1.6.12) gives

$$\begin{cases} -\dot{Z} = Z^2 + V''_{x,x}(q) \\ Z(0) = Z_0 = \mathrm{i}\mathbb{I} \end{cases}$$

that is exactly (1.6.4), that means the solution is simply the matrix $Z(t)$ given by (1.6.5):

$$Z(t) = \mathcal{S}(t)_* Z_0$$

From (1.6.10) we get another Cauchy problem

$$\begin{cases} \dfrac{\dot{\alpha}}{\alpha} = -\dfrac{1}{2}\mathrm{tr}\, Z \\ \alpha(0) = (\det \mathrm{Im}\, Z_0)^{1/4} \\ -\dot{\Theta} - \langle p, \dot{q} \rangle = \frac{|p|^2}{2} + V(q) \\ \Theta(0) = 0 \end{cases} \tag{1.6.14}$$

If we pose

$$\Theta(t) = \int_0^t \langle p(s), \dot{q}(s) \rangle - h(q(s), p(s)) ds$$

and

$$\alpha(t) = (\det \mathrm{Im}\, Z_0)^{1/4} e^{-\frac{1}{2}\int_0^t \mathrm{tr}\,[\mathcal{S}(s)_* Z_0] ds}$$

then we get a solution of (1.6.14). So, since we have found $\alpha(t), (q(t), p(t)), Z(t), \Theta(t)$, we can construct $\psi(t,x)$ and we have

$$\psi(t,x) = e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} \left(\frac{1}{\pi\varepsilon}\right)^{n/4} \alpha(t) e^{\frac{\mathrm{i}}{\varepsilon}\langle Z(t)(x-q(t)), x-q(t)\rangle/2} e^{\frac{\mathrm{i}}{\varepsilon}\langle p(t), x-q(t)\rangle} \tag{1.6.15}$$

Note that a priori, we don't know how $Z(t)$ evolves in time, but we can rewrite $Z(t) = \mathrm{Re}\, Z(t) + \mathrm{i}\,\mathrm{Im}\, Z(t)$ and the wave function takes the form

$$\psi(t,x) = e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} \left(\frac{1}{\pi\varepsilon}\right)^{n/4} \alpha(t)\widetilde{a}\left(\frac{x-q(t)}{\sqrt{\varepsilon}}\right) e^{\frac{\mathrm{i}}{\varepsilon}\langle \mathrm{Re}\, Z(t)(x-q(t)), x-q(t)\rangle/2} e^{\frac{\mathrm{i}}{\varepsilon}\langle p(t), x-q(t)\rangle} \tag{1.6.16}$$

$$= \left(\frac{1}{\pi\varepsilon}\right)^{n/4} a\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} e^{\frac{\mathrm{i}}{\varepsilon}\left[\langle p(t), x-q(t)\rangle + \frac{1}{2}\langle V(t)(x-q(t)), x-q(t)\rangle\right]} = e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} \psi^{a(t)}_{(q(t),p(t))} \tag{1.6.17}$$

where we have posed

$$\begin{cases} \widetilde{a}\left(\dfrac{x-q(t)}{\sqrt{\varepsilon}}\right) = e^{\frac{1}{2\varepsilon}\langle \operatorname{Im} Z(t)(x-q(t)), x-q(t)\rangle} \\ \\ a\left(t, \dfrac{x-q(t)}{\sqrt{\varepsilon}}\right) := \alpha(t)\widetilde{a}\left(\dfrac{x-q(t)}{\sqrt{\varepsilon}}\right) \\ \\ V(t) := \operatorname{Re} Z(t) \end{cases} \tag{1.6.18}$$

and clearly $a \in \mathcal{S}(\mathbb{R}^n)$.
(ii) Now we compute the remainder $R\psi(t,x)$. We have

$$\left(\mathrm{i}\varepsilon\frac{\partial}{\partial t} - H\right)\psi(t,x) = R\psi(t,x)$$

where R is defined as

$$R = V(x) - \sum_{|\beta|\leq 2} \frac{V^{\beta}(q(t))}{\beta!}(x-q(t))^{\beta} = O((x-q(t))^3) \tag{1.6.19}$$

and

$$R\psi(t,x) = \left[V(x) - \sum_{|\beta|\leq 2} \frac{V^{\beta}(q(t))}{\beta!}(x-q(t))^{\beta}\right] \alpha(t) e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x,t)}$$

where $\varphi(x,t) = \Theta(t) + \langle p(t), x-q(t)\rangle + \frac{1}{2}\langle Z(t)(x-q(t)), x-q(t)\rangle$. We want to prove that

$$\|R\psi(t,\cdot)\|_{L^2} \leq C\varepsilon^{3/2} |\operatorname{Im} Z(t)|_{\infty}^{-3/2} \tag{1.6.20}$$

We start observing that

$$|R\psi(t,x)|^2 \leq C(\varepsilon)|\alpha(t)|^2 \left|R^2 e^{\frac{\mathrm{i}}{\varepsilon}\varphi(t,x)}\right| \left|e^{\frac{\mathrm{i}}{\varepsilon}\varphi(t,x)}\right| \tag{1.6.21}$$

where $C(\varepsilon)$ is the normalization constant (of the initial coherent state). Now we prove that

$$|R^2 e^{\frac{\mathrm{i}}{\varepsilon}\varphi(t,x)}| \leq C\varepsilon^3 |\operatorname{Im} Z(t)|^3 \tag{1.6.22}$$

holds true. To prove it we will use Lemma (A.2.2). To this end note that

$$\operatorname{Im}\varphi(x,t) = \frac{1}{2}\langle \operatorname{Im} Z(t)(x-q(t)), (x-q(t))\rangle$$

and that $\operatorname{Im}\varphi(t,x) \geq 0$ from the fact that $Z(t) \in \Sigma_d$ because $\mathcal{S}(t) \in \operatorname{Sp}(d,\mathbb{R})$ and $Z_0 \in \Sigma_d$ (see Theorem 1.5.12). Clearly the amplitute $a(t,x)$ of $R^2\psi(t,x)$ is of order $O((x-q(t))^6)$ (and so for the x variable the condition (A.2.4) is satisfied), while in the t variable we have to put the term

$|\mathrm{Im}\, Z(t)|_\infty$. Finally we have to set $N = \frac{6}{2} = 3$ (because $\mathrm{Im}\,\varphi$ is of order 2 in $x - q(t)$). So we get

$$|a(t,x)| \le \widetilde{C} |\, \mathrm{Im}\, Z(t)|_\infty^{-3}$$

and applying Lemma (A.2.2) we get

$$\left| R^2 \psi(t,x) \right| \le \bar{C} \varepsilon^3 |\, \mathrm{Im}\, Z(t)|_\infty^{-3}$$

uniformly in x as required. Next we look at the term $\left| e^{\frac{i}{\varepsilon}\varphi(t,x)} \right|$ in (1.6.21).

$$\left| e^{\frac{i}{\varepsilon}\varphi(t,x)} \right| = e^{-\frac{1}{\varepsilon}\langle \mathrm{Im}\, Z(t)(x-q(t)) | x - q(t) \rangle}$$

that is a Gaussian centered on $q(t)$. So we have that (1.6.21) becomes

$$|R\psi(t,x)|^2 \le C(\varepsilon) \varepsilon^3 |\, \mathrm{Im}\, Z(t)|_\infty^{-3} |\alpha(t)|^2 e^{-\frac{1}{\varepsilon}\langle \mathrm{Im}\, Z(t)(x-q(t)) | x - q(t) \rangle}$$

and taking the square root of the integral over $\mathbb{R}^n$ on both sides, we have

$$\|R\psi(t,\cdot)\|_{L^2} \le C \varepsilon^{3/2} |\, \mathrm{Im}\, Z(t)|_\infty^{-3/2}$$

The last step is to use Lemma 1.6.1: we easily get

$$\left\| \phi(t,\cdot) - e^{\frac{i}{\varepsilon}\Theta(t)} \psi^{a(t)}_{(q(t),p(t))}(\cdot) \right\|_{L^2} \le C t \varepsilon^{1/2} \sup_{s \in [0,t]} |\, \mathrm{Im}\, Z(s)|_\infty^{-3/2}$$

□

1.6.1 Ehrenfest time

To better understand the error term in Theorem (1.6.3), one has to find a bound for $|\,\mathrm{Im}\, Z(t)|$.

The pendulum

We consider as an example the case of the classical pendulum. Let $(x, \xi) \in \mathbb{R}^2$ and let

$$h(x,\xi) = \frac{\xi^2}{2} + \cos x - 1$$

with $x \in [0, 2\pi]$, be the classical Hamiltonian. Then the Quantum Mechanical operator associated to h is

$$H = -\frac{\varepsilon}{2}\Delta + \cos x - 1$$

and suppose that we want to construct an approximate solution to (1.6.3) where we choose the coherent state centered on an equilibrium point $(q(0), p(0))$. It is trivial to see that there are two equilibrium points given by $(0,0)$ (unstable) and $(\pi, 0)$ (stable). In both cases we will have

$(q(t), p(t)) = (q(0), p(0))$ since these two points are equilibria. We now try to find estimates for $\operatorname{Im} Z(t)$.

(i) Stable case: in this situation one has that the matrix $\mathcal{S}$ in (1.6.6) is given by

$$\begin{cases} \dot{\mathcal{S}} = \begin{pmatrix} \dot{S}_{11} & \dot{S}_{12} \\ \dot{S}_{21} & \dot{S}_{22} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \cos\pi & 0 \end{pmatrix} \mathcal{S} = \begin{pmatrix} S_{21} & S_{22} \\ -S_{11} & -S_{12} \end{pmatrix} \\ \mathcal{S}(0) = \mathbb{I} \end{cases} \tag{1.6.23}$$

and we can easily determine all the entries of the matrix. One ends up with

$$\mathcal{S}(t) = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix} \tag{1.6.24}$$

and the function $Z(t)$ will be given by

$$Z(t) = (S_{21} + \mathrm{i}S_{22})(S_{11} + \mathrm{i}S_{12})^{-1} = (\sin t + \mathrm{i}\cos t)(\cos t - \mathrm{i}\sin t)^{-1} \tag{1.6.25}$$

$$= (\sin t + \mathrm{i}\cos t)(\cos t + \mathrm{i}\sin t) = \mathrm{i} \tag{1.6.26}$$

since $Z_0 = \mathrm{i}$. We have $|\operatorname{Im} Z(t)| = 1$ and the error in the estimate (1.6.8) will be $C\varepsilon^{1/2}t$. In this case the approximation will be accurate up to times of order $t \sim O(\varepsilon^{-1/2})$.

(ii) Unstable case: in this case the matrix of the linearized system is

$$\mathcal{S}(t) = \begin{pmatrix} \cosh t & \sinh t \\ \sinh t & \cosh t \end{pmatrix} \tag{1.6.27}$$

and $Z(t)$ is given by

$$\begin{aligned} Z(t) &= (S_{21} + \mathrm{i}S_{22})(S_{11} + \mathrm{i}S_{12})^{-1} = (\sinh t + \mathrm{i}\cosh t)(\cosh t + \mathrm{i}\sinh t)^{-1} \\ &= \frac{2\sinh t\cosh t}{\sinh^2 t + \cosh^2 t} + \mathrm{i}\frac{\cosh^2 t - \sinh^2 t}{\sinh^2 t + \cosh^2 t} \\ &= \tanh 2t + \mathrm{i}\frac{1}{\sinh^2 t + \cosh^2 t} \end{aligned} \tag{1.6.28}$$

and so

$$|\operatorname{Im} Z(t)|^{-3/2} = (\sinh^2 t + \cosh^2 t)^{3/2} = (\cosh 2t)^{3/2} \leq e^{3t} \tag{1.6.29}$$

Then the error term will be $C\varepsilon^{1/2}te^{3t}$ and the approximation will be good up to times smaller than

$$t \leq W\left(\frac{C}{\sqrt{\varepsilon}}\right) \tag{1.6.30}$$

where $W(x)$ is the so called Lambert W-function (i.e. the inverse of the function $f(x) = xe^x$). Taking ε small enough one has that $W(1/\sqrt{\varepsilon})$ is well approximated by $\log(1/\sqrt{\varepsilon})$, so our approximation is good up to times

$$t \sim \ln \frac{1}{\varepsilon} \tag{1.6.31}$$

The general case

Here we want to find an estimate for the matrix norm $|\operatorname{Im} Z(t)|$ in the more general case where

$$h(x,\xi) = \frac{|\xi|^2}{2} + V(x) \tag{1.6.32}$$

with the corresponding Quantum Mechanical operator

$$H = -\frac{\varepsilon^2}{2}\Delta + V(x)$$

Now we suppose that $V(x)$ has a stable equilibrium point (q_s, p_s) and/or an unstable equilibrium point (q_u, p_u).

Theorem 1.6.4. *Let $h(x,\xi)$ as in (1.6.32)*

(i) If (q_s, p_s) is a stable equilibrium point and we consider the Cauchy problem (1.6.3) with initial datum $\psi_{(q_s,p_s)}(x)$, then $\sup_{s\in[0,t]} |\operatorname{Im} Z(s)|_\infty^{-3/2} \leq C$ where $C \in \mathbb{R}$ is a constant. In this case the approximation of Theorem (1.6.3) is valid up to times of order $t \sim 1/\sqrt{\varepsilon}$.

(ii) If (q_u, p_u) is an unstable equilibrium point and we consider the Cauchy problem (1.6.3) with initial datum $\psi_{(q_u,p_u)}(x)$, then $\sup_{s\in[0,t]} |\operatorname{Im} Z(s)|_\infty^{-3/2} \leq e^{3\lambda t}$ where $\lambda > 0$ is a constant. In this case the approximation of Theorem (1.6.3) is valid up to times of order $t \sim \frac{1}{\lambda}\ln\frac{1}{\varepsilon}$.

Proof. First of all note that in (i) and (ii) the matrix of the system (1.6.6) has constant coefficients so the solution will be

$$\mathcal{S}(t) = e^{Mt} \tag{1.6.33}$$

where

$$M = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ -V''(q^*) & \mathbb{O} \end{pmatrix} \tag{1.6.34}$$

and $q^* = q_u, q_s$. $\mathcal{S}(t)$ is a symplectic matrix and can be decomposed as in (1.5.6) so that

$$\mathcal{S}(t) = \begin{pmatrix} A & \mathbb{O} \\ \mathbb{O} & A^{-T} \end{pmatrix} \begin{pmatrix} \mathbb{I} & \mathbb{O} \\ B & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbb{O} & -\mathbb{I} \\ \mathbb{I} & \mathbb{O} \end{pmatrix} = \begin{pmatrix} \mathbb{O} & -A \\ A^{-T} & -A^{-T}B \end{pmatrix} \tag{1.6.35}$$

and the matrix $Z(t)$ will be given by

$$Z(t) = (S_{21} + \mathrm{i}S_{22})(S_{11} + \mathrm{i}S_{12}) = (A^{-T} - \mathrm{i}A^{-T}B)(-\mathrm{i}A)^{-1} = (A^{-T} - \mathrm{i}A^{-T}B)(\mathrm{i}A^{-1}) \tag{1.6.36}$$

Then the imaginary part of $Z(t)$ is

$$\operatorname{Im} Z(t) = (AA^T)^{-1}$$

and considering its norm

$$|\operatorname{Im} Z(t)| = |(AA^T)^{-1}| \geq |AA^T|^{-1}$$

Finally

$$\sup_{s\in[0,t]} |\operatorname{Im} Z(s)|^{-3/2} \leq |AA^T|^{3/2} \leq |A|^3 \leq \sup_{s\in[0,t]} |\mathcal{S}(s)|^3$$

where the last inequality comes from the fact that A is a block of $\mathcal{S}$ and so the norm of $\mathcal{S}$ will be bigger than the norm of A. Then both (i) and (ii) are easily derived observing that $\mathcal{S}(t)$ is the matrix of the linearized flow.
(i) Since we are linearizing around a stable equilibrium point $|\mathcal{S}(s)| \leq C^{1/3}$ for all $s \in [0,t]$, where C is a constant and so $\sup_{s\in[0,t]} |\operatorname{Im} Z(s)|^{-3/2} \leq C$. From this we will have that our approximation is valid up to

$$C\varepsilon^{1/2} t \leq 1 \Rightarrow t \sim \frac{1}{\sqrt{\varepsilon}}$$

(ii) The point (q_u, p_u) in an unstable equilibrium, so $\sup_{s\in[0,t]} |\mathcal{S}(s)| \leq ce^{\lambda t}$ where $\lambda > 0$ is the greatest Lyapunov exponent of the classical system and $c \in \mathbb{R}_{>0}$ is a constant. This implies that the error term will remain small until

$$C\varepsilon^{1/2} t e^{3\lambda t} \leq 1$$

and this is solved by

$$t \leq \frac{1}{\lambda} W\left(\frac{C\lambda}{\sqrt{\varepsilon}}\right)$$

where W is W-Lambert function. The last expression can be well approximated by

$$t \sim \frac{1}{\lambda} \ln \frac{1}{\varepsilon}$$

□

We want to make some remarks on the proof of the previous theorem: first of all if we look in the details of the proof we can see that the same argument can be used if we center the Coherent State $\psi_{(q,p)}(x)$ on a general point (q,p) of the phase space. For example in [Pau07b], the author suggests that $|\operatorname{Im} Z(t)|^{-3/2} \leq e^{3\mu(x,\xi)t}$ where $\mu(x,\xi) \geq 0$ is an α-Hölder function (with $\alpha > 0$) depending on the point of the phase space (x,ξ) and the "goal" is to find the smallest μ.
The second observation is that we have find two different scales of times for which the approximation is good:

$$\begin{cases} t \sim \dfrac{1}{\sqrt{\varepsilon}} \\ \\ t \sim \dfrac{1}{\lambda} \ln \dfrac{1}{\varepsilon} \end{cases}$$

We will call these times Ehrenfest times.

Definition 1.6.5. *The Ehrenfest time $t_E(\varepsilon)$ is defined as*

$$t_E(\varepsilon) \sim \begin{cases} \frac{1}{\sqrt{\varepsilon}} & \text{in the stable case} \\ \\ \frac{1}{\lambda}\ln\frac{1}{\varepsilon} & \text{in the unstable case} \end{cases} \tag{1.6.37}$$

1.6.2 Spreading of wave packets

Following the work of Comberscue and Robert in [CR97] we choose $\alpha = (q,p)$ (a fixed point of the classical motion), and we take as initial datum the coherent state $\varphi_\alpha = D(\alpha)\psi_{(0,0)}$ centered on (q,p), where

$$\begin{cases} \alpha = \dfrac{q + \mathrm{i}p}{\sqrt{2\varepsilon}} \\ \\ a = \dfrac{X + \mathrm{i}P}{\sqrt{2\varepsilon}}, \quad a^\dagger = \dfrac{X - \mathrm{i}P}{\sqrt{2\varepsilon}} \\ \\ D(\alpha) = \exp(\bar{\alpha}a^\dagger - \alpha a) \end{cases}$$

and $\psi_{(0,0)}(x) = (\pi\varepsilon)^{-n/4}\exp(-|x|^2/(2\varepsilon))$. We want to measure the spreading of the wave packets so we define

$$\begin{aligned} S(t) :=& \Big\langle D(-\alpha)\psi(t,x) \Big| \sum_{j=1}^{n}(a_j^\dagger a_j + a_j a_j^\dagger) D(-\alpha)\psi(t,x)\Big\rangle \\ =& \|aD(-\alpha)\psi(t,x)\|^2 + \|a^\dagger D(-\alpha)\psi(t,x)\|^2 \end{aligned}$$

where $\psi(t,x) = e^{-\frac{\mathrm{i}}{\varepsilon}Ht}\varphi_\alpha(x)$.

Lemma 1.6.6. $S(0) = n$.

Proof. One has

$$\begin{aligned} S(0) &= \left\langle D(-\alpha)\psi(0,x) \middle| \sum_{j=1}^{n}(a_j^\dagger a_j + a_j a_j^\dagger) D(-\alpha)\psi(0,x) \right\rangle \\ &= \left\langle D(-\alpha)D(\alpha)\psi_{(0,0)} \middle| \sum_{j=1}^{n}(a_j^\dagger a_j + a_j a_j^\dagger) D(-\alpha)D(\alpha)\psi_{(0,0)} \right\rangle \\ &= \sum_{j=1}^{n}\langle a_j\psi_{(0,0)}|a_j\psi_{(0,0)}\rangle + \langle a_j^\dagger\psi_{(0,0)}|a_j^\dagger\psi_{(0,0)}\rangle \\ &= \sum_{j=1}^{n}\|a_j\psi_{(0,0)}\|^2 + \|a_j^\dagger\psi_{(0,0)}\| \end{aligned}$$

Next we calculate

$$\begin{aligned} a_j^\dagger \psi_{(0,0)}(x) &= \frac{X_j - \mathrm{i}P_j}{\sqrt{2\varepsilon}} \left(\frac{1}{(\pi\varepsilon)^{n/4}} e^{-\frac{|x|^2}{2\varepsilon}} \right) \\ = \sqrt{\frac{1}{2\varepsilon}} \frac{1}{(\pi\varepsilon)^{n/4}} x_j e^{-\frac{|x|^2}{2\varepsilon}} &+ \sqrt{\frac{1}{2\varepsilon}} \frac{1}{(\pi\varepsilon)^{n/4}} x_j e^{-\frac{|x|^2}{2\varepsilon}} \\ &= \sqrt{\frac{2}{\varepsilon}} \frac{1}{(\pi\varepsilon)^{n/4}} x_j e^{-\frac{|x|^2}{2\varepsilon}} \end{aligned}$$

and finally we get

$$\begin{aligned} \left\| a_j^\dagger \psi_{(0,0)} \right\|^2 = \left\langle a_j^\dagger \psi_{(0,0)} \middle| a_j \psi_{(0,0)} \right\rangle &= \frac{2}{\varepsilon} \frac{1}{(\pi\varepsilon)^{n/2}} \int_{\mathbb{R}^n} x_j^2 e^{-\frac{|x|^2}{\varepsilon}} dx \\ = \frac{2}{\varepsilon} \frac{1}{(\pi\varepsilon^{n/2})} \int_{\mathbb{R}} x_j^2 e^{-\frac{|x|^2}{\varepsilon}} dx_j &= \frac{2}{\varepsilon} \frac{\varepsilon}{2} = 1 \end{aligned}$$

In the same way one can show that

$$a_j \psi_{(0,0)}(x) = 0$$

and so we get

$$S(0) = \sum_{j=1}^{n} \|a_j \psi_{(0,0)}\|^2 + \|a_j^\dagger \psi_{(0,0)}\| = n$$

as required. □

Our aim is to compute

$$\Delta S(t) := S(t) - S(0) = S(t) - n$$

that is the dispersion (or the spreading) of the wave packet. We first calculate

$$T(t) := \left\langle D(-\alpha)\Phi(t) \middle| \sum_{j=1}^{n} (a_j^\dagger a_j + a_j a_j^\dagger) D(-\alpha)\Phi(t) \right\rangle$$

where $\Phi(t)$ is the approximant of $\Psi(t)$ given by

$$\Phi(t) = e^{i\delta_t/\varepsilon} \Phi_0(t) = e^{i\delta_t/\varepsilon} D(\alpha) U_0(t) \Psi_0$$

We get

$$T(t) = n + 2\|aU_0(t)\Psi_0\|^2 = n + \mathrm{tr}\,(Z_t^* Z_t)$$

where $(Z_t)_{jk} = (u_k + iv_k)_j$, u and v solve

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = JM_t \begin{pmatrix} u \\ v \end{pmatrix}$$

and M_t is the Hessian of H at $(q_t, p_t) = \alpha_t$. Moreover we call λ the Lyapunov exponent relative to the fixed point α. One of the main results of the paper is the following Theorem.

Theorem 1.6.7. *We have the asymptotics* $\Delta S(t) = \Delta T(t) + O(\varepsilon^\alpha)$ *if one of the following conditions is fulfilled:*

(i) $\lambda \le 0$ *("stable case") and* $0 \le t \le \varepsilon^{\alpha - 1/2}$

(ii) $\lambda > 0$ *("unstable case") and* $\exists \varepsilon' > \varepsilon$ *such that* $0 \le t \le ((1-2\varepsilon')/6\lambda)\log(1/\varepsilon)$

Proof. For the proof see [CR97]. □

In the same article there is another important result that tells us how fast the spreading is.

Corollary 1.6.8. *Assume that* H *is time independent and the greatest Lyapunov exponent is* $\lambda > 0$*. Then* $\Delta S(t) \sim e^{2\lambda t}$ *as* $t \to +\infty$ *and* $\varepsilon \to 0$ *as long as* $t[\log(1/\varepsilon)]^{-1}$ *stays small enough.*

In the following our aim will be to recover a similar result in our construction. We start this part observing that, using Theorem 1.6.3, we can construct a wave packet that approximates the solution of Schrödinger equation and has the following form

$$\psi(t,x) = e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} \left(\frac{1}{\pi\varepsilon}\right)^{n/4} \alpha(t) e^{\frac{\mathrm{i}}{\varepsilon}\langle Z(t)(x-q(t)), x-q(t)\rangle/2} e^{\frac{\mathrm{i}}{\varepsilon}\langle p(t), x-q(t)\rangle} \tag{1.6.38}$$

and, if we consider the probability density, we have

$$|\psi(t,x)|^2 \sim e^{\frac{1}{\varepsilon}\langle \operatorname{Im} Z(t)(x-q(t)), x-q(t)\rangle} \tag{1.6.39}$$

Now we give the following proposition.

Proposition 1.6.9. *The variance* σ *of the probability distribution (1.6.39) grows exponentially fast, i.e.* $\sigma \sim e^{kt}$ *where* $k > 0$ *is a constant, for* $t \to +\infty$ *and* $\varepsilon \to 0$ *as long as* $t[\log(1/\varepsilon)]^{-1}$ *stays small enough.*

Proof. The variance σ of the probability distribution in (1.6.39) is

$$\sigma(t) = \sqrt{\frac{\varepsilon}{2 \operatorname{Im} Z(t)}}$$

It is clear that, since (1.6.38) is an approximation valid up to times of order $t \sim t_E(\varepsilon) = \frac{1}{\lambda}\ln\frac{1}{\varepsilon}$, that we can "push" $t \to +\infty$ only if $t[\log(1/\varepsilon)]^{-1}$ stays small enough. Under this assumption we rewrite

$$\sigma(\varepsilon, t) = \varepsilon^{1/2}(2\operatorname{Im} Z(t))^{-1/2} \sim \varepsilon^{1/2} e^{\lambda t}$$

and putting $t \sim \frac{1}{\lambda}\ln\frac{1}{\varepsilon}$ we have

$$\sigma(\varepsilon) \sim \frac{1}{\sqrt{\varepsilon}} \to +\infty$$

for $\varepsilon \to 0$. This means that the gaussian start spreading exponentially fast in time as long as the condition $t[\log(1/\varepsilon)]^{-1} << 1$ is fullfilled. □

An example of the spreading of the wave packet

To clarify the problem of the spreading of the wave packet, we make a new example. Consider the following quantum mechanical operator

$$H = -\frac{\varepsilon^2}{2}\Delta + x^2(x^2-1)$$

where $x \in \mathbb{R}$. We know that approximating quantum evolution with a generalized coherent state makes the classical Hamiltonian "appear"

$$h(q,p) = \frac{p^2}{2} + x^2(x^2-1) \tag{1.6.40}$$

The graph of the double well and the phase-space contour plot can be seen in Figure 1.1.

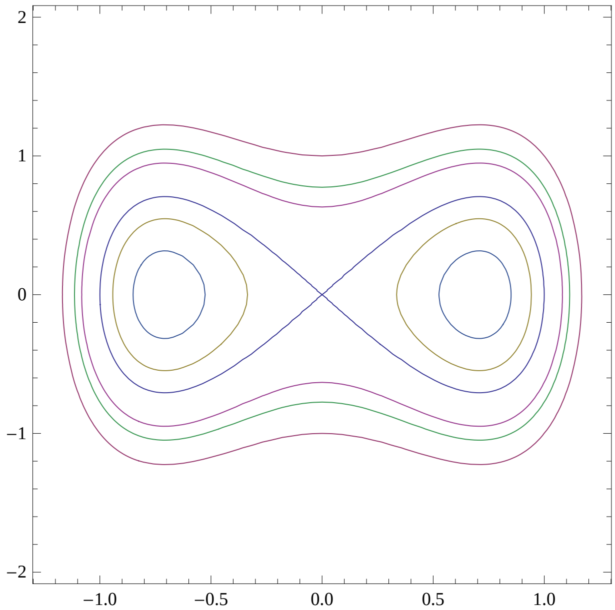

Figure 1.1: The phase portrait of the Hamiltonian in (1.6.40)

We consider as initial coherent state the following wave function

$$\psi_{(0,0)}(x) = \left(\frac{1}{\pi\varepsilon}\right)^{1/4} e^{\frac{\mathrm{i}}{2\varepsilon}\langle Z_0 x, x\rangle}$$

where $Z_0 = \mathrm{i}\mathbb{I}$ (that is a coherent state centered on the unstable equilibrium point $(0,0)$). We know from Theorem 1.6.3 that quantum evolution can be approximated by

$$\widetilde{\phi}(t,x) = \left(\frac{1}{\pi\varepsilon}\right)^{1/4} e^{\frac{\mathrm{i}}{\varepsilon}\langle Z(t)x,x\rangle}$$

since $(q(t),p(t)) = (0,0)$. We want to understand what happen at different "fractions" of

Eherenfest time: in particular we want to understand how the density spreads in time. Again we must compute $\operatorname{Im} Z(t)$ and, in order to do so, we must solve

$$\begin{pmatrix} \dot{S}_{11} & \dot{S}_{12} \\ \dot{S}_{21} & \dot{S}_{22} \end{pmatrix} = \begin{pmatrix} S_{21} & S_{22} \\ 2S_{11} & 2S_{12} \end{pmatrix}$$

with the initial condition $\mathcal{S}(0) = \mathbb{I}$. It is easy to find

$$\mathcal{S}(t) = \begin{pmatrix} \cosh\sqrt{2}t & \frac{1}{\sqrt{2}}\sinh\sqrt{2}t \\ \frac{2}{\sqrt{2}}\sinh\sqrt{2}t & \cosh\sqrt{2}t \end{pmatrix} \tag{1.6.41}$$

so that

$$Z(t) = \frac{\frac{\sqrt{2}}{2}\sinh\sqrt{2}t + \mathrm{i}\cosh\sqrt{2}t}{\cosh\sqrt{2}t + \mathrm{i}\frac{1}{\sqrt{2}}\sinh\sqrt{2}t} \tag{1.6.42}$$

and after some easy computations

$$Z(t) = \frac{2}{\sqrt{2}} \frac{\sinh\sqrt{2}t\cosh\sqrt{2}t}{1+\frac{3}{2}\sinh^2\sqrt{2}t} + \mathrm{i}\frac{1}{1+\frac{3}{2}\sinh^2\sqrt{2}t} \tag{1.6.43}$$

that implies that the imaginary part of the function $Z(t)$ is

$$\operatorname{Im} Z(t) = \frac{1}{1+\frac{3}{2}\sinh^2\sqrt{2}t}$$

Note that $\sup_{s\in[0,t]} |\operatorname{Im} Z(s)|_\infty^{-3/2} = |\operatorname{Im} Z(t)|_\infty^{-3/2} \leq e^{3\sqrt{2}t}$ so, in this example we can put $\lambda = \sqrt{2}$. Moreover the real part of $Z(t)$ is bounded: $|\operatorname{Re} Z(t)|_\infty \leq C$. The graphs of the functions $|\operatorname{Im} Z(t)|_\infty^{-3/2}$ and $|\operatorname{Re} Z(t)|_\infty$ are shown in Figure 1.2.

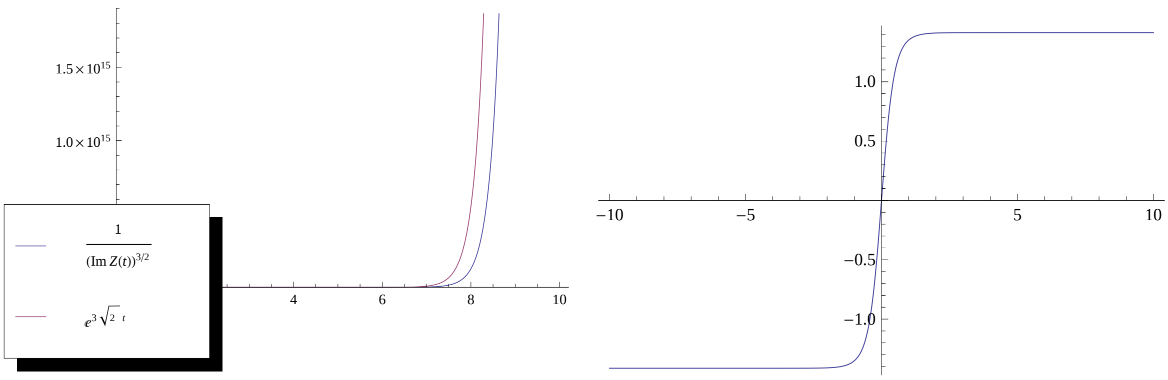

Figure 1.2: The plots of $(\operatorname{Im} Z(t))^{-3/2}$ (on the left) and of $\operatorname{Re} Z(t)$ (on the right)

We proceed as before: we compute the double of the variance of the probability distribution

$$|\psi(t,x)|^2 \sim \exp\left(-\frac{x^2}{\varepsilon(1+\frac{3}{2}\sinh^2\sqrt{2}\,t)}\right)$$

that is

$$2\sigma = 2\sqrt{\frac{\varepsilon}{2\,\mathrm{Im}\,Z(t)}} \tag{1.6.44}$$

It is easy to see that $2\sigma(t) \sim O(1)$ for $t \sim \frac{1}{2\sqrt{2}}\ln\frac{1}{\varepsilon}$, i.e. for $t \sim \frac{1}{2}t_E$. This means in particular that the semiclassical wave function is completely spread (over the unstable manifold) after half of Eherenfest time: we have recovered a result of Paul that can be found in [Pau09].

1.6.3 The limit $t \to \infty$

In this part we will study the limit for $t \to \infty$, for the approximate solutions of the Schrödinger equation as in Theorem 1.6.3. It is clear from the proof of that Theorem, that the approximation is of order $\varepsilon^{\frac{1}{2}}$ only if $t < \log\frac{1}{\varepsilon}$. In particular we will write $\lim_{\varepsilon t}$ for the "mixed" limit $\lim_{\varepsilon\to 0, t\to\infty}$ under the condition that $t\left(\log\frac{1}{\varepsilon}\right)^{-1}$ stays small enough (as in Corollary 1.6.8 or Proposition 1.6.9). For example, if we write the time as a function of ε, we can require that

$$\lim_{\varepsilon\to 0}\frac{t(\varepsilon)}{\log\frac{1}{\varepsilon}} = 0$$

So we proceed with the following definition.

Definition 1.6.10. *We define*

$$\lim_{\varepsilon t} f(\varepsilon;t) := \lim_{\varepsilon\to 0} f(\varepsilon;t(\varepsilon))$$

where the function $t(\varepsilon)$ satisfies

$$\lim_{\varepsilon\to 0}\frac{t(\varepsilon)}{\log\frac{1}{\varepsilon}} = 0$$

under the conditions:

(a) $\lim_{\varepsilon\to 0} t(\varepsilon) = +\infty$

(b) $t(\varepsilon) < E_{t(\varepsilon)}$ *for all* $\varepsilon > 0$ *and* $E_{t(\varepsilon)}$ *is the Ehrenfest time.*

Given a Gaussian coherent state $\psi_{(q,p)}(x)$, it is possible to rewrite it as

$$\psi_{(q,p)}(x) = A(x)e^{\frac{i}{\varepsilon}S(x)} \tag{1.6.45}$$

where

$$\begin{cases} A(x) = \frac{1}{(\pi\varepsilon)^{n/4}}e^{-\frac{(x-q)^2}{2\varepsilon}} \\ S(x) = \langle p, x-q\rangle \end{cases}$$

(we have omitted the (q, p)-dependence on $S(x)$ and $A(x)$ to lighten the notations). Now we try to solve the Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t\psi(t,x) = H\psi(t,x) \\ \psi^0(x) = \psi_{(q,p)}(x) \end{cases} \tag{1.6.46}$$

and using (1.6.45) in (1.6.46), we get the following system of PDEs

$$\begin{cases} \partial_t S + h(x, \nabla S) = \varepsilon^2 \frac{\Delta A}{A} \\ S(0,x) = \langle p, x-q\rangle \\ \partial_t(A^2) + \operatorname{div}(A^2\nabla S) = 0 \\ A(0,x) = \frac{1}{(\pi\varepsilon)^{n/4}} e^{-\frac{(x-q)^2}{2\varepsilon}} \end{cases} \tag{1.6.47}$$

that we will call Madelung system of PDEs and we will study in some more details in the following chapters. We note here that when $\varepsilon = 0$, the previous system of PDEs becomes

$$\begin{cases} \partial_t S + h(x, \nabla S) = 0 \\ S(0,x) = \langle p, x-q\rangle \\ \partial_t(A^2) + \operatorname{div}(A^2\nabla S) = 0 \\ A(0,x) = \delta_q(x) \end{cases}$$

Now we recall the result of Theorem 1.6.3: we can construct a semiclassical wave function $\psi^{\alpha(t),V(t)}_{(q(t),p(t))}$ such that

$$\left\| e^{-\frac{\mathrm{i}}{\varepsilon}tH}\psi_{(q,p)}(x) - e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)}\psi^{\alpha(t),V(t)}_{(q(t),p(t))}(x) \right\|_{L^2} \leq Cte^{\lambda t}\varepsilon^{1/2}$$

and

$$\psi^{\alpha(t),V(t)}_{(q(t),p(t))}(x) = \left(\frac{1}{\pi\varepsilon}\right)^{n/4} \alpha(t) e^{\frac{\mathrm{i}}{\varepsilon}\Theta(t)} e^{\frac{\mathrm{i}}{\varepsilon}\langle Z(t)(x-q(t)), x-q(t)\rangle/2} e^{\frac{\mathrm{i}}{\varepsilon}\langle p(t), x\rangle}$$

where $V(t) = \operatorname{Re} Z(t)$. We know from the previous sections that an approximate solution to the first equation of (1.6.47) is given by

$$S(t,x) = \langle p(t), x\rangle + \int_0^t p(s)\dot{q}(s) - h(q(s),p(s))ds + \frac{1}{2}V(t) \tag{1.6.48}$$

Here we define

$$S(t,x) = \langle p(t), x\rangle + \Theta(t) + \frac{1}{2}V(t)$$

where $\Theta(t)$ is given by

$$\Theta(t) = \int_0^t p(s)\dot{q}(s) - h(q(s),p(s))ds$$

Moreover note that $\lim_{t\to\infty} \frac{V(t)}{t} = 0$ since $|\operatorname{Re} Z(t)|_\infty < +\infty$. We want to perform the limit $\lim_{t\to\infty} \frac{S(t,x)}{t}$, but we can do this limit under the condition of the Definition 1.6.10, since the semiclassical approximation must be valid.
Let us suppose that the Hamiltonian function has one of the following forms:

(i) $h(q,p) = |p|^2/2 + V(q)$;

(ii) $h(q,p) = h(p)$;

(iii) $h(q,p) = \tilde{h}(p) + \delta f(q,p)$, with $0 < \delta \ll 1$ small enough, if the dimension of the cotangent fiber bundle is 2 or 4.

and that we can associate the corresponding Lagrangian function (using the Legendre transform). In the first case the energy level sets $h(q,p) = E$ are compact. In particular we have that the classical motion $(q(t), p(t))$ will be confined in this set. In the other cases we will have:

(ii) h is integrable, so

$$\begin{cases} p(t) = p(0) \\ q(t) = \omega t + q(0) \end{cases}$$

(iii) h is quasi-integrable and the dimension is low, so

$$\|p(t) - p(0)\| \leq O(\sqrt{\varepsilon})$$

there is not Arnol'd diffusion.

In all the previous cases

(i) from the fact that the energy levels are compact then $\|p(t)\| < +\infty$ and one gets

$$\lim_{\varepsilon t} \frac{S(t,x)}{t} = \lim_{\varepsilon t} \frac{\langle p(t), x\rangle + \Theta(t) + \frac{1}{2}V(t)}{t} = \lim_{\varepsilon t} \frac{\Theta(t)}{t}$$

(ii) from the fact that $p(t) = p(0)$, we have

$$\lim_{\varepsilon t} \frac{S(t,x)}{t} = \lim_{\varepsilon t} \frac{\langle p(t), x\rangle + \Theta(t)}{t} = \lim_{\varepsilon t} \frac{\langle p(0), x\rangle + \Theta(t) + \frac{1}{2}V(t)}{t} = \lim_{\varepsilon t} \frac{\Theta(t)}{t}$$

(iii) without Arnol'd diffusion: $p(t) \leq p(0) \pm C\sqrt{\varepsilon}$ and:

$$\lim_{\varepsilon t} \frac{S(t,x)}{t} = \lim_{\varepsilon t} \frac{\langle p(t), x\rangle + \Theta(t) + \frac{1}{2}V(t)}{t} = \lim_{\varepsilon t} \frac{\Theta(t)}{t}$$

In all three cases one has the following equalities:

$$\begin{aligned}\lim_{\varepsilon t}\frac{S(t,x)}{t}=\lim_{\varepsilon t}\frac{\Theta(t)}{t}&=\lim_{\varepsilon t}\frac{1}{t}\int_0^t[p(s)\dot{q}(s)-h(q(s),p(s))]ds\\&=\lim_{\varepsilon t}\frac{1}{t}\int_0^t l(q,\dot{q})ds\end{aligned}$$

where $l(x,\dot{x})$ is the Lagrangian associated to h. It follows that

$$\lim_{\varepsilon t}\frac{S(t,x)}{t}\geq\lim_{t\to\infty}\frac{1}{t}\inf\Big\{\int_0^t l(q(s),\dot{q}(s))ds\Big\}=c[0]$$

where $c[0]$ is Mañé critical value relative to h.

Remark 1.6.11 In fact the same result holds even in the case when

$$\lim_{t\to\infty}\frac{\|p(t)\|}{t}=0$$

So it is possible to have Arnol'd diffusion: we need only that the velocity of the moments to be small enough.

1.7 Coherent States and defect measures

The fact that the Coherent States are the most "classical" object in Quantum Mechanics is reaffirmed by the following theorem.

Theorem 1.7.1. *Let $h(x,\xi)$ be a symbol and $H=h(x,\varepsilon D)$ its standard quantization. Then considering the set of coherent states*

$$\psi_{(q,p)}(\varepsilon,x)=\left(\frac{1}{\pi\varepsilon}\right)^{n/4}e^{-\frac{|x-q|^2}{2\varepsilon}}e^{\frac{\mathrm{i}}{\varepsilon}\langle p,x-q\rangle}\tag{1.7.1}$$

one has

$$\lim_{\varepsilon\to0}\langle H\psi_{(q,p)}(\varepsilon,x)|\psi_{(q,p)}(\varepsilon,x)\rangle=h(q,p)\tag{1.7.2}$$

Proof. We compute

$$\begin{aligned}&\langle h(x,\varepsilon D)\psi_{(q,p)}(\varepsilon,x)|\psi_{(q,p)}(\varepsilon,x)\rangle=\\&=\left(\frac{1}{2\pi\varepsilon}\right)^n\iiint_{\mathbb{R}^{3n}}h(x,\xi)e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle}\psi_{(q,p)}(\varepsilon,y)\bar{\psi}_{(q,p)}(\varepsilon,x)\,dyd\xi dx\\&=\frac{2^{n/2}}{(2\pi\varepsilon)^{3n/2}}\iiint_{\mathbb{R}^{3n}}h(x,\xi)e^{\frac{\mathrm{i}}{\varepsilon}(\langle x-y|\xi\rangle+\langle y-q|p\rangle-\langle x-q|p\rangle)}e^{-\frac{1}{2\varepsilon}(|y-q|^2+|x-q|^2)}\,dyd\xi dx\\&=\frac{2^{n/2}}{(2\pi\varepsilon)^{3n/2}}\iiint_{\mathbb{R}^{3n}}h(x,\xi)e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi-p\rangle}e^{-\frac{1}{2\varepsilon}(|y-q|^2+|x-q|^2)}\,dyd\xi dx\end{aligned}\tag{1.7.3}$$

Now fix (x, ξ) and calculate the integral in y

$$\begin{aligned}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi-p\rangle} e^{-\frac{1}{2\varepsilon}|y-q|^2}\,dy &= e^{\frac{\mathrm{i}}{\varepsilon}\langle x-q|\xi-p\rangle}\int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}\langle y|\xi-p\rangle} e^{-\frac{1}{2\varepsilon}|y|^2}\,dy\\ &= e^{\frac{\mathrm{i}}{\varepsilon}\langle x-q|\xi-p\rangle}\mathcal{F}\left(e^{-\frac{1}{2\varepsilon}|y|^2}\right)\left(\frac{\xi-p}{\varepsilon}\right)\\ &= (2\pi\varepsilon)^{n/2} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-q|\xi-p\rangle} e^{-\frac{1}{2\varepsilon}|\xi-p|^2}\end{aligned}$$

Going back to the mean value

$$\begin{aligned}\langle h(x,\varepsilon D)\psi_{(q,p)}(\varepsilon,x)|\psi_{(q,p)}(\varepsilon,x)\rangle &=\\ = \frac{2^{n/2}}{(2\pi\varepsilon)^n}\iint_{\mathbb{R}^{2n}} h(x,\xi) e^{\frac{\mathrm{i}}{\varepsilon}\langle x-q|\xi-p\rangle} e^{-\frac{1}{2\varepsilon}(|x-q|^2+|\xi-p|^2)}\,dxd\xi\\ h(q,p)\frac{2^{n/2}}{(2\pi\varepsilon)^n}\iint_{\mathbb{R}^{2n}} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-q|\xi-p\rangle} e^{-\frac{1}{2\varepsilon}(|x-q|^2+|\xi-p|^2)}\,dxd\xi + o(1)\\ = Ch(q,p) + o(1)\end{aligned}$$

The last step is to show that the constant C is equal to 1. But it is an easy computation, since

$$C = \frac{2^{n/2}}{(2\pi)^n}\iint_{\mathbb{R}^{2n}} e^{\mathrm{i}\langle x|\xi\rangle} e^{-\frac{1}{2}(|x|^2+|\xi|^2)}\,dxd\xi = 1$$

□

In the proof of the previous Theorem we showed that the measure associated to a coherent state of the form (1.7.1) is the Dirac measure $\delta_{(q,p)}$, since applying Theorem (B.4.2) we have

$$\lim_{\varepsilon\to 0}\langle H\psi_{(q,p)}(\varepsilon,x)|\psi_{(q,p)}(\varepsilon,x)\rangle = \int_{\mathbb{R}^{2n}} h(x,\xi)\,d\mu(x,\xi) = \int_{\mathbb{R}^{2n}} h(x,\xi)\,\delta_{(q,p)} = h(q,p) \qquad (1.7.4)$$

Moreover it is important to understand that coherent states are useful in "de-quantizing" simbols: given a quantized operator one can recover its classical symbol computing its mean value on coherent states. As we will see in next section coherent states are a particular subclass of Lagrangian states: these are the states that "concentrates" around a Lagrangian submanifold of the phase space.

1.8 Lagrangian states

Another example of a particular class of states is given by the functions of the form

$$e^{\frac{i}{\varepsilon}\varphi(x)}$$

with $\varphi(x)$ is a real function, or by a linear superposition of these functions

$$\left(\frac{1}{2\pi\varepsilon}\right)^{n/2}\int_{\mathbb{R}^n} e^{\frac{i}{\varepsilon}\varphi(x,\theta)}a(x,\theta)d\theta$$

where $\operatorname{Im}\varphi(x,\theta)=0$. From the stationary phase method (see Appendix A.1), these functions are concentrated on the Lagrangian submanifold

$$\Lambda_\varphi=\{(x,\varphi'_x(x,\theta)):\varphi'_\theta(x,\theta)=0\}$$

1.8.1 Quantization of Lagrangian submanifold

We look for approximate solutions of the stationary Schrödinger equation

$$(H-E)\psi=0 \tag{1.8.1}$$

That means that we look for a function $\psi(\varepsilon,x)$ and $E(\varepsilon)$ such that

$$(H-E(\varepsilon))\psi(\varepsilon,x)=O(\varepsilon^N)$$

for $\varepsilon\to 0$ and some $N\in\mathbb{N}$. Following the classical WKB theory, we choose ψ of the form

$$\left(\frac{1}{2\pi\varepsilon}\right)^{n/2}\int_{\mathbb{R}^n} e^{\frac{i}{\varepsilon}\varphi(x,\theta)}a(\varepsilon,x,\theta)d\theta \tag{1.8.2}$$

where φ is a real valued function and $a(\varepsilon,x,\theta)$ has an asymptotic expansion of the form

$$a(\varepsilon,x,\theta)\sim\sum_{n=0}^{\infty}\varepsilon^n a_n(x,\theta)$$

for $\varepsilon\to 0$. We assume that $a(\varepsilon,x,\theta)$ has uniformly compact support in θ and $\varphi(x,\theta)$ is assumed to be smooth and non degenerate on the set $\{(x,\theta)|\varphi'_\theta(x,\theta)=0\}$. Moreover we assume that $E(\varepsilon)$ has the asymptotic expansion

$$E(\varepsilon)\sim\sum_{n=0}\varepsilon^n E_n$$

At the points x where $\varphi'_\theta(x,\theta)=0$ has only one solution $\theta(x)$ in a neighborhood of x, we can apply the method of stationary phase to get

$$\psi(\varepsilon,x)=e^{\frac{i}{\varepsilon}\varphi(x,\theta(x))}\tilde{a}(\varepsilon,x)$$

where

$$\tilde{a}(\varepsilon,x)=\frac{e^{i\frac{\pi}{4}\operatorname{sign}\varphi''_{\theta,\theta}(x,\theta(x))}}{|\det\varphi''_{\theta,\theta}(x,\theta(x))|^{1/2}}a_0(x,\theta(x))+O(\varepsilon)$$

The last expression holds true when x is a non degenerate point for $\varphi(x,\theta(x))$. If for a given x there is no θ with $(x,\theta)\in \operatorname{supp} a$ and for which φ is stationary, then

$$\psi(\varepsilon,x)=O(\varepsilon^{\infty})$$

We have to determine the action of the operator $\mathcal{H}$ on the oscillating function $e^{\frac{i}{\varepsilon}\varphi}a$.

Theorem 1.8.1. *Let H a pseudodifferential operator with symbol $h(\lambda,\xi,x)\in S^0(m_{a,b})$, and $a(x),\varphi(x)$ smooth functions with $\operatorname{Im}\varphi(x)\geq 0$; $a(x)$ is compactly supported. Then*

$$H(ae^{\frac{i}{\varepsilon}\varphi})(x)=b(\varepsilon,x)e^{\frac{i}{\varepsilon}\varphi(x)}+O(\varepsilon^{\infty})$$

and $b(\varepsilon,x)$ is given by

$$b(\varepsilon,x)=e^{i\varepsilon(\langle D_y,D_\xi\rangle+\frac{1}{2}\langle D_\xi,\varphi''(x)D_\xi\rangle)}e^{\frac{i}{\varepsilon}R(x,y)}\widetilde{h}\Big(\varepsilon;\xi+\varphi'(x),x+\frac{y}{2}\Big)a(x+y)|_{y=0,\xi=0} \tag{1.8.3}$$

where $\widetilde{h}$ is an almost analytic extension of the symbol h of H and R is given by

$$R(x,y)=\varphi(x+y)-\varphi(x)-\langle\varphi'(x),y\rangle-\frac{1}{2}\langle y,\varphi''(x)y\rangle$$

Proof. See [Dui96]. □

Note that the first two terms of the expansion $b\sim b_0+\varepsilon b_1+\varepsilon^2 b_2+\ldots$, are given by

$$b_0(x)=a_0(x)h_0(x,\varphi') \tag{1.8.4}$$

$$b_1(x)=a_1(x)h_0(x,\varphi')+a_0(x)h_1(x,\varphi')+\mathrm{i}\left(\partial_x a_0(x)\partial_\xi h_0(x,\varphi')+\frac{1}{2}a_0(x)\partial_x\partial_\xi h_0(x,\varphi')\right) \tag{1.8.5}$$
$$+\,\mathrm{i}\left(\frac{1}{2}a_0(x)\partial_\xi\varphi''\partial_\xi h_0(x,\varphi')\right)$$

Now if we use (1.8.2) in equation (1.8.1), we find

$$(H-E(\varepsilon))\psi(\varepsilon,x)=\left(\frac{1}{2\pi\varepsilon}\right)^{n/2}\int_{\mathbb{R}^n}e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x,\theta)}\left[b(\varepsilon,x,\theta)-E(\varepsilon)a(\varepsilon,x,\theta)\right]d\theta \tag{1.8.6}$$

and we require that $b(\varepsilon,x,\theta)-E(\varepsilon)a(\varepsilon,x,\theta)$ are $O(\varepsilon^{\infty})$ on the Lagrangian submanifold Λ_φ. This implies for the first two terms (using (1.8.4) and (1.8.5))

$$a_0h_0-E_0a_0=0 \tag{1.8.7}$$

$$a_1h_0+a_0h_1+\mathrm{i}\left(\partial_x a_0\partial_\xi h_0+\frac{1}{2}a_0\partial_x\partial_\xi h_0+\frac{1}{2}a_0\partial_\xi\varphi''\partial_\xi h_0\right)-E_0a_1-E_1a_0=0 \tag{1.8.8}$$

We can rewrite equation (1.8.7) as

$$h_0(x,\varphi'_x(x,\theta))=E_0 \tag{1.8.9}$$

that is an Hamilton-Jacobi equation for φ. From symplectic geometry and the theory of Hamilton-Jacobi equations, the set

$$\Lambda_\varphi = \{(x, \varphi'_x(x,\theta)) \,|\, \varphi'_\theta(x,\theta) = 0\} \tag{1.8.10}$$

is a Lagrangian submanifold of T^*X. Then the Hamilton-Jacobi equation (1.8.9) has a solution if there exists a Lagrangian submanifold of T^*X which is invariant under the Hamiltonian flow relative to X_{h_0}, the principal simbol of H.
Now if (1.8.9) is satisfied, then (1.8.8) becomes

$$a_0(h_1 - E_1) + \mathrm{i}\left(\partial_x a_0 \partial_\xi h_0 + \frac{1}{2} a_0 \partial_x \partial_\xi h_0 + \frac{1}{2} a_0 \partial_\xi \varphi'' \partial_\xi h_0\right) = 0 \tag{1.8.11}$$

and, using the fact that $\frac{1}{2}a_0\partial_x\partial_\xi h_0 + \frac{1}{2}a_0\partial_\xi\varphi''\partial_\xi h_0 = \frac{1}{2}a_0\frac{\partial}{\partial x}\partial_\xi h_0(x,\varphi')$, we get

$$a_0(h_1(x,\varphi'(x)) - E_1) + \mathrm{i}\left(\partial_x a_0(x,\theta)\partial_\xi h_0(x,\varphi'(x)) + \frac{1}{2}a_0(x,\theta)\frac{\partial}{\partial x}\partial_\xi h_0(x,\varphi'(x))\right) = 0 \tag{1.8.12}$$

We can think of a_0 as a half density on Λ: the Lie derivative of a half density $b(x)|dx|^{1/2}$ in the direction of the vector field X is given by

$$\mathcal{L}_X b(x)|dx|^{1/2} = \left(X(b) + \frac{1}{2}(\mathrm{div}X)b\right)|dx|^{1/2}$$

hence equation (1.8.12) becomes

$$\frac{1}{\mathrm{i}}\mathcal{L}_{X_{h_0}} a_0 - (h_1 - E_1)a_0 = 0 \tag{1.8.13}$$

once we interpret a_0 as a half density on Λ. Using Stokes theorem, we can find a necessary condition for the previous equation to be solvable:

$$E_1 = \int_\Lambda h_1 d\mu_\Lambda$$

1.9 Wick rotation, coherent states and Hamilton-Jacobi equation

In this section we want to point out a connection between weak solutions of Hamilton-Jacobi equation, coherent states and Wick rotation. The Wick rotation consists in the "complexification" of the time $t \mapsto it$ and it is equivalent to the complexification of $\varepsilon \mapsto \mathrm{i}\varepsilon$. So we introduce the parameter $\delta = \frac{1}{\mathrm{i}\varepsilon}$ and we look at the Schrödinger equation for $\delta \to \infty$ with δ in the set of real numbers (so we are considering ε purely imaginary). Schrödinger equation becomes

$$\frac{1}{\delta}\frac{\partial\psi}{\partial t}(t,x) = H_\delta\psi(t,x) \tag{1.9.1}$$

where H_δ is the operator $H_\delta = \frac{1}{2\delta^2}\Delta + V(x)$ (note the change of sign in front of the Laplacian). In the following $x \in X$ where X is a manifold. If we look for solution of (1.9.1) of the form

$$\psi(t,x) = \exp\left(-\delta S_\delta(t,x)\right) \tag{1.9.2}$$

(this is called Cole-Hopf transformation) we find that $S_\delta(t,x)$ must solve

$$\frac{\partial S_\delta}{\partial t} + h(x, \nabla_x S_\delta) = \frac{\Delta S_\delta}{2\delta} \tag{1.9.3}$$

where

$$h(x,p) = \frac{1}{2}|p|^2 + V(x) \tag{1.9.4}$$

We give the following definition of *viscosity solution* of Hamilton-Jacobi equation.

Definition 1.9.1. *A continuous function $S : \mathbb{R}_{>0} \times X \to \mathbb{R}$ is a viscosity solution of*

$$\frac{\partial S}{\partial t} + h(x, \nabla_x S) = 0 \tag{1.9.5}$$

if for every C^2 function φ the following conditions hold:

(i) S is a sub-solution: for all $(t,y) \in \mathbb{R}_{>0} \times X$ such that $S - \varphi$ has a local maximum, one has

$$\frac{\partial \varphi}{\partial t} + h(x, \nabla_x \varphi) \leq 0 \tag{1.9.6}$$

(ii) S is a super-solution: for all $(t,y) \in \mathbb{R}_{>0} \times X$ such that $u - \varphi$ has a local minimum, one has

$$\frac{\partial \varphi}{\partial t} + h(x, \nabla_x \varphi) \geq 0 \tag{1.9.7}$$

For $\delta \to \infty$ one obtains exactly the weak solutions of Hamilton-Jacobi equation (1.9.5). References are in [Lio83] or in [BD97]. Under some particular conditions on the Hamiltonian h, the stationary Hamilton-Jacobi equation

$$h(x, \nabla u) = E \tag{1.9.8}$$

selects an unique (weak) solution (see [AIPSM05] or the discussion in §4.4 below). From the work of Davini and Siconolfi [DS06] one has, choosing $X = \mathbb{T}^n$, that the solution $S(t,x)$ behaves for $t \to \infty$ as $S(t,x) \sim u(x) - ct$: this is a sort of "spreading" of the function S for large times. In the following we will try to connect this result with coherent states evolution. We start choosing as initial datum for (1.9.1) the "coherent state"

$$\psi(0,x) = \exp\left[-\delta\left(\frac{1}{2}\langle Z(x-q), x-q\rangle + \langle p, x-q\rangle\right)\right] \tag{1.9.9}$$

Then we proceed as in Section 1.6: we look for an approximate solution of (1.9.1) with a form strictly analogous to the already used for the standard Schrödinger equation (see Theorem 1.6.3)

$$\psi(t,x) = e^{-\delta\left[-\frac{1}{\delta}\ln\alpha(t)+\frac{1}{2}\langle Z(t)(x-q(t)),x-q(t)\rangle+\langle p(t),x-q(t)\rangle+\Theta(t)\right]} \tag{1.9.10}$$

and we find $(q(t),p(t)), Z(t), \alpha(t), \Theta(t)$ as before (that is, using a Taylor approximation up to $O(|x-q|^3)$) . The problem is that we don't know if the matrix $Z(t)$ has the same properties of the analogous matrix of coherent states: if so then we will have a spreading phenomena also in this case and a similar result to the one in [ISM09] (the exponential "spreading" of the function $S(t,x)$). This would provide another link between classical WKAM theory and Quantum Mechanics. Now we try to go further in this direction. First we define $\beta(t) = \ln\alpha(t)$ in (1.9.10), so that it becomes

$$\psi(t,x) = e^{-\delta\left[-\frac{1}{\delta}\beta(t)+\frac{1}{2}\langle Z(t)(x-q(t)),x-q(t)\rangle+\langle p(t),x-q(t)\rangle+\Theta(t)\right]}$$

and we compute $\frac{\partial\psi}{\partial t}$:

$$\begin{aligned}\frac{1}{\delta}\frac{\partial\psi}{\partial t}(t,x) = \frac{1}{\delta}\dot\beta(t) - \frac{1}{2}\langle\dot Z(t)(x-q(t))|(x-q(t))\rangle + \langle Z(t)\dot q(t)|x-q(t)\rangle - \\ -\langle\dot p(t)|x-q(t)\rangle + \langle p(t)|\dot q(t)\rangle - \dot\Theta(t)\end{aligned}$$

and $H_\delta\psi(t,x)$:

$$\begin{aligned}H_\delta\psi(t,x) = -\frac{1}{2\delta}\operatorname{tr} Z(t) + \frac{1}{2}\Big(p(t)+Z(t)(x-q(t))\Big)^2 + V(q(t)) + \\ +V'(q(t))(x-q(t)) + \frac{1}{2}V''(q(t))(x-q(t))^2\end{aligned}$$

Now comparing the two terms we get the following equations

$$\dot\beta(t) = -\frac{1}{2}\operatorname{tr} Z(t) \tag{1.9.11}$$

$$\langle p(t)|\dot q(t)\rangle - \dot\Theta(t) = \frac{|p(t)|^2}{2} + V(q(t)) \tag{1.9.12}$$

$$Z(t)\dot q(t) - \dot p(t) = Z(t)p(t) + V'(q(t)) \tag{1.9.13}$$

$$-\dot Z(t) = Z^2(t) + V''(q(t)) \tag{1.9.14}$$

We start our discussion from equation (1.9.13). It can be easily seen (again) that we can determine the function $(q(t),p(t))$ simply as the solution of Hamilton equations relative to the hamiltonian $h(q,p) = \frac{|p|^2}{2} + V(q)$. Next we look at equation (1.9.12): having $(q(t),p(t))$ we can easily find $\Theta(t)$. More precisely

$$\Theta(t) = \int pdq - hdt$$

(written in a compact form). Then equation (1.9.11) is easily solved by

$$\beta(t) = \ln\left(e^{-\frac{1}{2}\int_0^t \operatorname{tr}[\mathcal{S}(s)_* Z_0]ds}\right) \tag{1.9.15}$$

where $\mathcal{S}(t)$ is the (well-known) matrix solving (1.6.6) and the $*$ product is defined as in (1.6.5). The only difference with the work done in the previous section is in equation (1.9.14): we have to solve the following Cauchy problem

$$\begin{cases} -\dot{Z}(t) = Z^2(t) + V''(q(t)) \\ Z(0) = \mathbb{I} \end{cases}$$

and not

$$\begin{cases} -\dot{Z}(t) = Z^2(t) + V''(q(t)) \\ Z(0) = \mathrm{i}\mathbb{I} \end{cases}$$

Since the general solution to this problem is given by $Z(t) = \mathcal{S}(t)_* Z_0$, for $Z_0 = \mathbb{I}$ we have

$$Z(t) = \mathcal{S}(t)_* \mathbb{I} = (S_{21} + S_{22})(S_{11} + S_{12})^{-1} \tag{1.9.16}$$

and we can use again the decomposition of the matrix $\mathcal{S}$ we used in (1.5.6), so that

$$\mathcal{S}(t) = \begin{pmatrix} \mathbb{O} & -A \\ -A^T & -A^T B \end{pmatrix}$$

In this way we have from (1.9.16)

$$Z(t) = (A^{-T} - A^{-T}B)(-A)^{-1} = (A^{-T}BA^{-1} - A^{-T}A^{-1})$$

and applying the sup-norm to the matrix, we get

$$\begin{gathered} |Z(t)|_\infty = |A^{-T}BA^{-1} - A^{-T}A^{-1}|_\infty \le \\ \le |A^{-T}BA^{-1}|_\infty + |(AA^T)^{-1}|_\infty = |\operatorname{Re}\widetilde{Z}(t)|_\infty + |\operatorname{Im}\widetilde{Z}(t)|_\infty \end{gathered}$$

compare with (1.6.36), where $\widetilde{Z}(t)$ solves

$$\begin{cases} -\dot{\widetilde{Z}}(t) = \widetilde{Z}^2(t) + V''(q(t)) \\ \widetilde{Z}(0) = \mathrm{i}\mathbb{I} \end{cases} \tag{1.9.17}$$

We already know from section §1.6 that $|\operatorname{Re}\widetilde{Z}(t)|_\infty \le C$ and $|\operatorname{Im}\widetilde{Z}(t)|_\infty^{-3/2} \le e^{\lambda t}$. In the following 1-dimensional case we are able to get more precise results which appear in a good correspondence with the weak KAM description of the related classical Hamiltonian system.

The one dimensional case

To understand better the problem, we consider the one dimensional case. Moreover we set $(q(t), p(t)) = (q_u, p_u)$ an unstable equilibrium point and without loss of generality we can choose $(q_u, p_u) = (0, 0)$. We have that the matrix $Z(t)$ in this case is function that satisfies the following equation

$$-\dot{Z}(t) = Z^2(t) + V''(0) \tag{1.9.18}$$

where $V''(0)$ is a negative constant (since $(0, 0)$ is an unstable equilibrium point): we define $k_0 = V''(0)$. Now we write $Z(t) = X(t) + \mathrm{i}Y(t)$ and we get that the real and the imaginary part of $Z(t)$ satisfy

$$\begin{cases} \dot{X}(t) = Y^2(t) - X^2(t) - k_0 \\ \dot{Y}(t) = -2X(t)Y(t) \end{cases} \tag{1.9.19}$$

If we want to find equilibria we have to solve the system

$$\begin{cases} Y^2 - X^2 - k_0 = 0 \\ 2XY = 0 \end{cases}$$

that has as solutions the points $(\pm\sqrt{-k_0}, 0)$. We can easily look at the stability of these points: considering the linearized system around the equilibria we find that $(+\sqrt{-k_0}, 0)$ in an attractor while $(-\sqrt{-k_0}, 0)$ is a repeller. Moreover it is easy to understand that considering

$$\begin{cases} -\dot{Z}(t) = Z^2(t) + k_0 \\ Z(0) = 1 \end{cases}$$

then the solution $Z(t)$ is real and $Z(t) \to +\sqrt{-k_0}$ for $t \to +\infty$. Now we come back to the approximate solution $\widetilde{\psi}(t, x)$ of the real Schrödinger equation

$$\widetilde{\psi}(t, x) = e^{-\delta \widetilde{S}(t,x)}$$

where $\widetilde{S}(t, x)$ is given by

$$\widetilde{S}(t, x) = -\frac{1}{\delta}\beta(t) + \frac{1}{2}Z(t)(x - q(t))^2 + p(t)(x - q(t)) + \Theta(t) \tag{1.9.20}$$

and since $(q(t), p(t)) = (0, 0)$ we can rewrite

$$\widetilde{S}(t, x) = -\frac{1}{\delta}\beta(t) + \frac{1}{2}Z(t)x^2 + \Theta(t) \tag{1.9.21}$$

We consider the limit: $\lim_{t\to+\infty} \frac{\widetilde{S}(t,x)}{t}$. We have that

$$\lim_{t\to+\infty} \frac{-\beta(t)}{\delta\, t} = 0$$

because $\beta(t)$ for t running to $+\infty$ is going to a constant (see (1.9.15)), and moreover

$$\lim_{t\to+\infty} \frac{\Theta(t)}{t} = -c[0]$$

where $c[0]$ is the Mañé critical value (see Section 4.2). We obtain

$$\widetilde{S}(t,x) \overset{t\to+\infty}{\sim} \sqrt{-k_0}\, x^2 - c[0]t \tag{1.9.22}$$

that is we have, for t big enough, that the solution "splits" into a time component and a space component: this is similar to the result of [DS06]. In addition to this we have to notice that this splitting is exponentially fast and this is again similar to the result of [ISM09].

What we have presented here is still work in progress but we think that it is important to understand the relation between the *semiclassical limit* and the WKAM theory (presented in Chapter 4).

Chapter 2

WKB constructions of quasimodes

2.1 Quasimodes

Preliminaries

Definition 2.1.1. *Let $\mathcal{H}$ be an Hilbert space and H a self adjoint operaton on $\mathcal{H}$ with domain $D(\mathcal{H})$. A couple (ψ, E) with $\psi \in D(\mathcal{H})$, $\|\psi\| = 1$ (here $\|\cdot\|$ denotes the norm on the Hilbert space $\mathcal{H}$) and $E \in \mathbb{R}$ is called quasimode with error δ if*

$$(H - E)\psi = r, \quad \text{with } \|r\| \leq \delta \tag{2.1.1}$$

First of all we observe that:

(i) even if (ψ, E) is a quasimode with small error δ, ψ could be far away from an eigenfunction;

(ii) on the other hand if (ψ, E) is a quasimode then E is close to an eigenvalue.

Proposition 2.1.2. *Let (ψ, E) a quasimode with error δ and suppose that the spectrum of H is discrete in a neighbourhood of $[E - \delta, E + \delta]$. Then there is at least one eigenvalue of H in $[E - \delta, E + \delta]$.*

Proof. Let $\mathcal{R}_H(E) := (H - E)^{-1}$ be the resolvent. Then

$$\|\mathcal{R}_H(E)\| \leq \frac{1}{\operatorname{dist}(E, \operatorname{spec}(H))}$$

Now we choose $\widetilde{E} \notin \operatorname{spec}(H)$ close to E and we apply to (2.1.1) $\mathcal{R}_H(\widetilde{E})$

$$(H - \widetilde{E})^{-1}(H - E)\psi = (H - \widetilde{E})^{-1}\Big[(H - \widetilde{E})\psi + (\widetilde{E} - E)\psi\Big] = \mathcal{R}_H(\widetilde{E})r$$
$$\psi = \mathcal{R}_H(\widetilde{E})r - (\widetilde{E} - E)\mathcal{R}_H(\widetilde{E})\psi$$

Then we take the norm and we have

$$1 = \|\psi\| \leq \frac{\|r\|}{\mathrm{dist}(\widetilde{E}, \mathrm{spec}(H))} + \frac{|\widetilde{E} - E|}{\mathrm{dist}(\widetilde{E}, \mathrm{spec}(H))}$$
$$\mathrm{dist}(\widetilde{E}, \mathrm{spec}(H)) \leq \delta + |\widetilde{E} - E|$$

and letting $\widetilde{E} \to E$ we get the result. □

Quasimodes allows us to approximate well the spectrum of an operator but not its eigenfunctions, as the following example shows.

Remark 2.1.3 Consider $\psi = a_1\psi_1 + a_2\psi_2$ with $|a_1|^2 + |a_2|^2 = 1$ and ψ_1, ψ_2 two eigenfunctions of H. Then

$$(H - E)\psi = a_1(E_1 - E)\psi_1 + a_2(E_2 - E)\psi_2 = r$$

and $\|r\|^2 \leq (E_1 - E)^2 + (E_2 - E)^2$. If E_1 and E_2 are close to E then $\|r\|$ is small but this does not imply that ψ is close to ψ_1 or ψ_2.

One interesting property of quasimodes is that they evolve like eigenfunctions.

Theorem 2.1.4. *Let H be a semiclassical Hamiltonian, (ψ, E) a quasimode with error δ and let $\mathcal{U}(t) = e^{-\frac{i}{\varepsilon}tH}$. Then*

$$\|\mathcal{U}(t)\psi - e^{-\frac{i}{\varepsilon}tE}\psi\| \leq \delta\frac{t}{\varepsilon}$$

Proof.

$$\begin{aligned}
\mathcal{U}(t)\psi - e^{-\frac{i}{\varepsilon}tE}\psi &= e^{-\frac{i}{\varepsilon}tE}[e^{\frac{i}{\varepsilon}tE}\mathcal{U}(t)\psi - \psi] \\
&= -\frac{i}{\varepsilon}e^{-\frac{i}{\varepsilon}tE}\int_0^t i\varepsilon\partial_{t'}(e^{\frac{i}{\varepsilon}t'E}\mathcal{U}(t')\psi)dt' \\
&= -\frac{i}{\varepsilon}e^{-\frac{i}{\varepsilon}tE}\int_0^t e^{\frac{i}{\varepsilon}t'E}\mathcal{U}(t')(H - E)\psi dt'
\end{aligned}$$

Taking the norms

$$\|\mathcal{U}(t)\psi - e^{-\frac{i}{\varepsilon}tE}\psi\| \leq \frac{t}{\varepsilon}\|r\| = \delta\frac{t}{\varepsilon}$$

□

2.1.1 Lagrangian quasimodes

Consider the stationary Schrödinger equation

$$H(x, -i\varepsilon\nabla)\psi = E\psi$$

where $\psi(x) = a(x)e^{\frac{i}{\varepsilon}u(x)}$ where a and u are real functions with $u(x) = P \cdot x + v(x)$ and $H(x,p) = \frac{|p|^2}{2} + W(x)$. In details we have

$$-\frac{\varepsilon^2}{2}\Delta\psi + W\psi = E\psi \tag{2.1.2}$$

Proposition 2.1.5. $\psi = ae^{\frac{i}{\varepsilon}u}$ *solves the stationary Schrödinger equation if and only if the couple* (a,u) *solve the following system of equations:*

$$\begin{cases} H(x,\nabla u) = E + \frac{\varepsilon^2}{2}\frac{\Delta a}{a} \\ div(a^2\nabla u) = 0 \end{cases} \tag{2.1.3}$$

Proof.

$$\Delta\psi = \Big(\Delta a + \frac{2i}{\varepsilon}\nabla a \cdot \nabla u - \frac{1}{\varepsilon^2}a|\nabla u|^2 + \frac{i}{\varepsilon}a\Delta u\Big)e^{\frac{i}{\varepsilon}u}$$

Putting this expression in (2.1.2), we find

$$\Big(a\Big(\frac{|\nabla u|^2}{2} + W - E\Big) - \frac{\varepsilon^2}{2}\Delta a\Big) - i\varepsilon(2\nabla a \cdot \nabla u + a\Delta u) = 0$$

Setting to zero the real and the imaginary part, dividing and multiplying by a the first and the second equation respectively, we get (2.1.3). □

Remark 2.1.6 The condition $u(x) = P \cdot x + v(x)$ is required because we want ψ to be a Bloch wave function (i.e. $\psi = e^{\frac{i}{\varepsilon}P\cdot x}\widehat{\psi}$). This imply that the system (2.1.3) is transformed into

$$\begin{cases} H(x, P + \nabla v(x,P)) = E(P) + \frac{\varepsilon^2}{2}\frac{\Delta a}{a} \\ \mathrm{div}((P + \nabla v(x,P))a^2(x,P)) = 0 \end{cases}$$

Remark 2.1.7 We can restate everything saying that ψ solves the stationary Schrödinger equation if and only if the couple (a,u) solve

$$H(x,\nabla u) = E + \frac{\varepsilon^2}{2}\frac{\Delta a}{a}$$

and the following conditions holds:

(i) $\mathrm{div}(a^2\nabla u) = 0$

(ii) $\displaystyle\int_{\mathbb{T}^n} a^2 dx = 1$

2.1.2 Variational formulation

We write again $\psi(x) = a(x)e^{\frac{i}{\varepsilon}u(x)}$.

Definition 2.1.8. *We define the action of ψ as*

$$\widetilde{A}[\psi] := \int_{\mathbb{T}^n} \Big(-\frac{\varepsilon^2}{2}|\nabla a|^2 + \frac{a^2}{2}|\nabla u|^2 - Wa^2 \Big) dx$$

where ψ must satisfy:

(i) $div(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) = 0$

(ii) $\int_{\mathbb{T}^n} |\psi|^2 dx = 1$

$\widetilde{A}$ is called Guerra-Morato action functional (see [GM83]).

It is easy to verify that (i) is nothing but

$$\operatorname{div}(a^2\nabla u) = 0$$

and (ii) implies $\int_{\mathbb{T}^n} a^2 dx = 1$.

Definition 2.1.9. *We define*

$$j_{\widetilde{A}}(\tau) := \int_{\mathbb{T}^n} \Big(-\frac{\varepsilon^2}{2}|\nabla a(\tau)|^2 + \frac{a(\tau)^2}{2}|\nabla u(\tau)|^2 - Wa(\tau)^2 \Big) dx \tag{2.1.4}$$

as the functional $\widetilde{A}[\psi]$ evaluated on the variations $\{a(\tau), u(\tau)\}_{-1\leq\tau\leq 1}$ with $\{a(0), u(0)\} = \{a, u\}$.

The following proposition clarifies the connection with what we have done before.

Proposition 2.1.10. *ψ is a critical point for the functional $\widetilde{A}[\psi]$ if and only if the couple (a, u) solves*

$$H(x, \nabla u) = E + \frac{\varepsilon^2}{2}\frac{\Delta a}{a} \tag{2.1.5}$$

Proof. Clearly ψ is a critical point for $\widetilde{A}$ only if $j'(0) = 0$. Now we get

$$j'(0) = \int_{\mathbb{T}^n} -\varepsilon^2\nabla a\cdot\nabla a' + aa'|\nabla u|^2 + a^2\nabla u\cdot\nabla u' - 2Waa'dx$$

Differentiating with respect to τ and posing $\tau = 0$ in the conditions (i) and (ii) of the definition of $\widetilde{A}$, we have

(i) $\operatorname{div}(2aa'\nabla u + a^2\nabla u') = 0$

(ii) $\int_{\mathbb{T}^n} 2aa'\nabla u + a^2\nabla u' dx = 0$

Integrating on $\mathbb{T}^n$ (i) multiplied by v and adding to it (ii) multiplied by P, we get:

$$\begin{aligned}0 &= \int_{\mathbb{T}^n} v \operatorname{div}(2aa'\nabla u + a^2\nabla u')dx + \int_{\mathbb{T}^n} P\cdot(2aa'\nabla u + a^2\nabla u')dx \\ &= \int_{\mathbb{T}^n} \nabla v\cdot(2aa'\nabla u + a^2\nabla u')dx + \int_{\mathbb{T}^n} P\cdot(2aa'\nabla u + a^2\nabla u')dx \\ &= \int_{\mathbb{T}^n} (\nabla v + P)\cdot(2aa'\nabla u + a^2\nabla u')dx = \int_{\mathbb{T}^n} \nabla u\cdot(2aa'\nabla u + a^2\nabla u')dx\end{aligned}$$

that is

$$\int_{\mathbb{T}^n} a^2\nabla u\cdot\nabla u' dx = -\int_{\mathbb{T}^n} 2aa'|\nabla u|^2 dx$$

Substituting this expression in $j'(0)$, one has

$$j'(0) = \int_{\mathbb{T}^n} -\varepsilon^2\nabla a\cdot\nabla a' - aa'|\nabla u|^2 - 2Waa'dx$$

and integrating by parts:

$$\int_{\mathbb{T}^n} -\varepsilon^2\nabla a\cdot\nabla a' dx = \int \varepsilon^2 a'\Delta a\, dx$$

The expression for j' becomes

$$j'(0) = \int_{\mathbb{T}^n} 2a'\left(\frac{\varepsilon^2}{2}\Delta a - \left(a\frac{|\nabla u|^2}{2} + Wa\right)\right)dx$$

Differentiating $\int_{\mathbb{T}^n} a^2 dx = 1$ with respect to τ and letting $\tau = 0$, we get

$$\int_{\mathbb{T}^n} a' a\, dx = 0$$

that is $j'(0) = 0$ if and only if

$$\frac{\varepsilon^2}{2}\Delta a - \left(a\frac{|\nabla u|^2}{2} + Wa\right) = -Ea$$

or, in other words,

$$\frac{\varepsilon^2}{2}\Delta a + Ea = \left(\frac{|\nabla u|^2}{2} + W\right)$$

From the fact that we must have $a > 0$, we have

$$H(x,\nabla u) = \frac{|\nabla u|^2}{2} + W = E + \frac{\varepsilon^2}{2}\frac{\Delta a}{a}$$

□

Remark 2.1.11 In conclusion we can restate everything in this way: $\psi(x) = a(x)e^{\frac{i}{\varepsilon}u(x)}$ solves the stationary Schrödinger equation if and only if the couple (a, u) solves the system (2.1.3) if and only if the couple (a, u) is stationary for the functional $\widetilde{A}$.

2.1.3 Evans' method

In his recent article [Eva07], Evans looks for a quantum version of WKAM theorem. He proceed in this way: he defines a "quantum" action functional and costructs some weak critical points for this action. It is easy to see that this action functional is the convex analog of Guerra-Morato action functional. Then he proves that the wave functions, constructed with these critical points, are approximate solutions of the Schrödinger stationary equation.

Definition 2.1.12. *The action functional for the wave function ψ is*

$$A[\psi] := \int_{\mathbb{T}^n} \frac{\varepsilon^2}{2}|\nabla\psi|^2 - W|\psi|^2 dx \tag{2.1.6}$$

where ψ satisfies the following:

(i) $\int_{\mathbb{T}^n} |\psi|^2 dx = 1$*;*

(ii) $\int_{\mathbb{T}^n} (\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) \cdot \nabla\phi \, dx = 0$ *for all* $\phi \in C^1(\mathbb{T}^n)$*;*

(iii) $\frac{\varepsilon}{2i}\int_{\mathbb{T}^n} \bar{\psi}\nabla\psi - \psi\nabla\bar{\psi} \, dx = V \in \mathbb{R}^n$*.*

If we consider again wave functions in polar form, i.e.

$$\psi(x) = a(x)e^{\frac{i}{\varepsilon}u(x)}$$

where $u(x) = P \cdot x + v(x)$, the action can be rewritten as

$$A[\psi] := \int_{\mathbb{T}^n} \Big(\frac{\varepsilon^2}{2}|\nabla a|^2 + \frac{a^2}{2}|\nabla u|^2 - Wa^2\Big)dx \tag{2.1.7}$$

and the conditions (i)-(iii) becomes

1. $\int_{\mathbb{T}^n} a^2 dx = 1$;
2. $\operatorname{div}(a^2\nabla u) = 0$;
3. $\int_{\mathbb{T}^n} a^2\nabla u \, dx = V$

Proceding as before, we give the following definition.

Definition 2.1.13.

$$j_A(\tau) := \int_{\mathbb{T}^n} \Big(\frac{\varepsilon^2}{2}|\nabla a(\tau)|^2 + \frac{a(\tau)^2}{2}|\nabla u(\tau)|^2 - W a(\tau)^2\Big) dx \tag{2.1.8}$$

is the functional $A[\psi]$ evaluated on the variations $\{a(\tau), u(\tau)\}_{-1\leq\tau\leq 1}$ where $\{a(0), u(0)\} = \{a, u\}$.

Theorem 2.1.14. *$j'(0) = 0$ for all the variations if and only if*

$$H(x, \nabla u) = E - \frac{\varepsilon^2}{2}\frac{\Delta a}{a} \tag{2.1.9}$$

Proof. The proof is the same of (2.1.5). □

We consider now the dual problems:

$$\begin{cases} -\frac{\varepsilon^2}{2}\Delta w + \varepsilon P\cdot\nabla w - W w = E_0 w \\ w \ \ \mathbb{T}^n\text{-periodic} \end{cases} \tag{2.1.10}$$

$$\begin{cases} -\frac{\varepsilon^2}{2}\Delta w^* - \varepsilon P\cdot\nabla w^* - W w^* = E_0 w^* \\ w^* \ \ \mathbb{T}^n\text{-periodic} \end{cases} \tag{2.1.11}$$

where $E_0 = E_0(\varepsilon, P)$ is the principal eigenvalue. Using Cole-Hopf transform

$$\begin{cases} w = e^{-v/\varepsilon} \\ w^* = e^{v^*/\varepsilon} \end{cases}$$

we get the following two problems

$$\begin{cases} -\frac{\varepsilon}{2}\Delta v + \frac{1}{2}|P + \nabla v|^2 + W = \bar{H}_\varepsilon(P) \\ v \ \ \mathbb{T}^n\text{-periodica} \end{cases} \tag{2.1.12}$$

$$\begin{cases} \frac{\varepsilon}{2}\Delta v^* + \frac{1}{2}|P + \nabla v^*|^2 + W = \bar{H}_\varepsilon(P) \\ v^* \ \ \mathbb{T}^n\text{-periodica} \end{cases} \tag{2.1.13}$$

where we have defined

$$\bar{H}_\varepsilon(P) := \frac{|P|^2}{2} - E_0(\varepsilon, P) \tag{2.1.14}$$

First of all we show that the principal eigenvalue $-E_0$ is precisely the energy E in 2.1.9.

Proposition 2.1.15. *The value E in (2.1.9) is equal to $-E_0$, i.e.*

$$E = -E_0$$

Proof. It is quite easy to prove: setting $P = 0$ in (2.1.12) and (2.1.13) we get

$$\begin{cases} -\frac{\varepsilon}{2}\Delta v + \frac{1}{2}|\nabla v|^2 + W = -E_0 \\ \frac{\varepsilon}{2}\Delta v^* + \frac{1}{2}|\nabla v^*|^2 + W = -E_0 \end{cases}$$

and using the definitions of u and a: $u(x) = \frac{v+v^*}{2}$, $a(x) = e^{\frac{v^*-v}{\varepsilon}}$ and substituting them into (2.1.9) one gets:

$$E = \Big[-\frac{\varepsilon}{4}\Delta v + \frac{1}{4}|\nabla v|^2 + \frac{1}{2}W\Big] + \Big[\frac{\varepsilon}{4}\Delta v^* + \frac{1}{4}|\nabla v^*|^2 + \frac{1}{2}W\Big]$$

and the conclusion follows. □

Remark 2.1.16 Evans is able to prove that

$$\bar{H}_\varepsilon(P) \leq \bar{H}(P) \leq \bar{H}_\varepsilon(P) + O(\varepsilon)$$

when $\varepsilon \to 0$. In other words

$$\lim_{\varepsilon\to 0} \bar{H}_\varepsilon(P) = \bar{H}(P)$$

for all $P \in \mathbb{R}^n$ where

$$\bar{H}(P) = \frac{1}{2}|\nabla u|^2 + W$$

for almost all $x \in \mathbb{T}^n$ (this means that $\bar{H}$ is the homogeneization of H) and $u = P \cdot x + v$. From min-max formula

$$\bar{H}(P) = \inf_{v\in C^1(\mathbb{T}^n)} \max_{x\in\mathbb{T}^n} \Big\{\frac{1}{2}|P + \nabla v|^2 + W(x)\Big\}$$

we get

$$\bar{H}(0) = \max_{x\in\mathbb{T}^n} W(x)$$

$$\bar{H}_\varepsilon(0) = -E_0(\varepsilon, 0)$$

and so

$$E_0(\varepsilon, 0) \to \min_{x\in\mathbb{T}^n}\{-W(x)\}$$

in the limit $\varepsilon \to 0$.

2.2 WKB constructions of quasimodes

First examples

In this section we follow [BB97].

On the real line

We consider stationary Schrödinger equation on $\mathbb{R}$

$$-\frac{\varepsilon^2}{2}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x)$$

for energy values $E \in I =]E_-, E_+[$. We suppose that in the interval I the level sets $\{\frac{p^2}{2} + V = E\}$ are periodic orbits. We choose two points $x_0 < x_1$ such that $V(x_i) = E$ (that corresponds to the caustics of the Lagrangian $\{H(x,p) = E\}$) and we look for solutions in the interval $]x_0, x_1[$ of the following form

$$\psi(x) = a(x)e^{\frac{i}{\varepsilon}S(x)}$$

Substituting in the Schrödinger equation such a function, we find that the phase $S(x)$ must satisfy the following Hamilton-Jacobi equation

$$\frac{|\partial_x S(x)|^2}{2} + V(x) = E \tag{2.2.1}$$

It is a well known fact that a solution of the previous equation is given by

$$S(x, x_0; E) = \pm\int_{x_0}^{x}\sqrt{2(E - V(y))}\,dy$$

or, equivalently, by

$$S(x_1, x; E) = \pm\int_{x}^{x_1}\sqrt{2(E - V(y))}\,dy$$

(where $x \in]x_0, x_1[$ and up to an additive constant). Moreover we find as a solution for the continuity equation the following amplitude

$$a(x) = \frac{C}{\sqrt{\partial_x S(x)}} = \frac{C}{\sqrt{p(x)}}$$

where we have identified the momentum $p(x)$ with $\partial_x S$. We have that the phase is a multivalued function and, in particular, we can write

$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left(Ae^{\frac{i}{\varepsilon}\int_x^{x_1}p(y)dy} + Be^{-\frac{i}{\varepsilon}\int_x^{x_1}p(y)dy}\right) \tag{2.2.2}$$

If $x < x_0$ or $x > x_1$ then $p(x) = i|p(x)|$ and in particular, for $x > x_1$ (i.e. in the classically forbidden region),

$$\psi(x) = \frac{1}{\sqrt{|p(x)|}}Ce^{-\frac{1}{\varepsilon}\int_{x_1}^{x}|p(y)|dy} \tag{2.2.3}$$

It is clear that in x_0 and in x_1 the two wave functions must coincide (paying attentio to the fact that in those points the semiclassical solution is not well defined because $p(x) = 0$). Using Taylor expansion in $x = x_1$, Schrödinger equation becomes

$$\frac{d^2\psi}{dx}(x) = \frac{2}{\varepsilon^2}(x - x_1)\partial_x V(x_1)\psi(x)$$

and translating x_1 in the origin, we get

$$\partial^2_{xx}\psi(y) = y\psi(y)$$

where we have posed $\frac{2}{\varepsilon^2}\partial_x V(0) = \alpha^3$ and $\alpha x = y$. The solution (for $y << 0$) of this equation is given by the so called Airy function

$$\mathrm{Ai}(y) \simeq |y|^{-1/4}\sin\Big(\frac{2}{3}|y|^{3/2} + \frac{1}{4}\pi\Big)$$

while for $y >> 0$ we have

$$\mathrm{Ai}(y) \simeq \frac{1}{2}y^{-1/4}e^{-\frac{2}{3}y^{3/2}}$$

Equalizing the first with (2.2.2) and the second with (2.2.3), one gets $B = -A = iCe^{i\frac{\pi}{4}}$ and ψ in the interior of the potential well becomes

$$\psi(x) = \frac{2C}{\sqrt{p(x)}}\sin\Big(\frac{1}{\varepsilon}\int_x^{x_1} p(y)dy + \frac{\pi}{4}\Big) \tag{2.2.4}$$

Proceeding analogously for x_0 (and considering the fact that $\partial_x V(x_0) < 0$) we have

$$\psi(x) = \frac{2\widetilde{C}}{\sqrt{p(x)}}\sin\Big(\frac{1}{\varepsilon}\int_{x_0}^{x} p(y)dy + \frac{\pi}{4}\Big) \tag{2.2.5}$$

For $x \in]x_0, x_1[$ we must have

$$C\sin\Big(\frac{1}{\varepsilon}\int_x^{x_1} p(y)dy + \frac{\pi}{4}\Big) = \widetilde{C}\sin\Big(\frac{1}{\varepsilon}\int_{x_0}^{x} p(y)dy + \frac{\pi}{4}\Big)$$
$$-\frac{1}{\varepsilon}\int_x^{x_1} p(y)dy - \frac{\pi}{4} + (n+1)\pi = \frac{1}{\varepsilon}\int_{x_0}^{x} p(y)dy + \frac{\pi}{4}$$

$$\frac{1}{\varepsilon}\int_{x_0}^{x_1} p(y)dy = \Big(n + \frac{1}{2}\Big)\pi \tag{2.2.6}$$

The equation (2.2.6) is called quantization condition (for energetic levels in a smooth potential well on the points x_0 and x_1). In a compact form

$$\frac{1}{\varepsilon}\oint pdx = \Big(n + \frac{1}{2}\Big)\pi$$

Suppose that $V(x_0) = +\infty$. Then the quantization condition changes: $\psi(x_1) = 0$ and so

$$\sin\Big(\frac{1}{\varepsilon}\int_{x_0}^{x_1} p(y)dy + \frac{\pi}{4}\Big) = 0$$

that gives us a different quantization condition

$$\frac{1}{\varepsilon}\int_{x_0}^{x_1} p(y)dy = \Big(n + \frac{3}{4}\Big)\pi$$

The potential "barrier" $V(x_0) = +\infty$ has added the phase $\frac{\pi}{2}$.

WKB on the torus: EKB

As we saw in the previous section, the action $S(x, x_0; E)$ is a multivalued function: it is made up by two components (two branches) and this is reflected in the wave function $\psi(x)$ showing two exponential terms of the form $\exp(\pm iS/\varepsilon)$. But this fact can be expressed in another way: the two branches represents the trajectory of the particle in the phase space and to every point on this curve must be associated an unique value of the momentum p_x. So, on this curve, the semiclassical wave function must be simply:

$$\psi(x, E) = \frac{1}{\sqrt{2\pi\varepsilon}}\Big|\frac{\partial^2 S(x, E)}{\partial E \partial x}\Big|^{1/2} \exp(iS(x, E)/\varepsilon)$$

Denote with ΔS the change in the phase after a full cycle. At each turning point we get an additional phase of $-\frac{\pi}{2}$ (because of the change of sign), and so one must have

$$\frac{1}{\varepsilon}\Delta S - 2\frac{\pi}{2} = 2n\pi$$

because of the single-valuedness. If the turning points are μ we get

$$\frac{1}{\varepsilon}\Delta S - \mu\frac{\pi}{2} = 2n\pi$$

and, since $\Delta S = 2\int pdq$ is the phase over the period, we have

$$\oint pdq = \Big(n + \frac{\mu}{4}\Big)\pi\varepsilon, \qquad n = 0, 1, 2, \dots$$

.

2.2.1 Near a minimum of the potential

We assume in the following that $V \in C^\infty(\mathbb{R}^n)$ admits a local non degenerate minimum in 0. We suppose (eventually changing the coordinates) that

(H1) $V(0) = 0$;

(H2) $V'(0) = 0$

(H3) $V''(0) > 0$

where $V''(0)$ is the Hessian of V in 0. We look for a formal solution of the following type

$$\psi(x, \varepsilon) = a(x, \varepsilon)e^{-\frac{\varphi(x)}{\varepsilon}}$$

Before starting the computations we need two proposition in order to solve the eikonal equation and the transport equations that we will find.

Proposition 2.2.1 ([Hel88]). *Assume (H1),(H2) and (H3) hold. Moreover assume that*

$$V''(0) = \begin{pmatrix} \mu_1 & 0 & \dots & 0 \\ 0 & \mu_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mu_n \end{pmatrix} \tag{2.2.7}$$

with $\mu_j > 0$ for all j and let $E_0 = \min V$. Then there exists an unique positive function $\varphi \in C^\infty(\mathbb{R}^n)$ defined in a neighborhood U of 0 such that

$$\frac{1}{2}|\nabla\varphi|^2 = (V - E_0) \tag{2.2.8}$$

in U and

$$\varphi(x) - \varphi_0(x) = O(|x|^3) \tag{2.2.9}$$

where

$$\varphi_0(x) = \sum_{i=1}^{n} \sqrt{\mu_i}\,\frac{x_i^2}{2}$$

Proof. We determine $\varphi(x)$ as the generating function of a Lagrangian submanifold

$$\Lambda^+ = \{(x, \varphi(x)), x \in W\}$$

where W is a neighborhood of 0 lying in $q^{-1}(0)$ where $q(x,\xi) = -p(x,\xi) = \frac{|\xi|^2}{2} - (V - E_0)$. In a neighborhood of $(0,0)$ in $T^*\mathbb{R}^n$ we have

$$q(x,\xi) = \frac{\xi^2}{2} - \sum_j \mu_j \frac{x_j^2}{2} + O(|(x,\xi)|^3)$$

and the vector field is given by

$$X_H = \sum_j \xi_j \frac{\partial}{\partial x_j} + \sum_j \mu_j x_j \frac{\partial}{\partial \xi_j} + O(|(x,\xi)|^2)$$

and its linear part is

$$Y_0 = \sum_j \xi_j \frac{\partial}{\partial x_j} + \sum_j \mu_j x_j \frac{\partial}{\partial \xi_j}$$

The matrix associated is

$$A = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ V''(0) & \mathbb{O} \end{pmatrix}$$

that has $\pm\sqrt{\mu_j}$ for $j = 1, \dots, n$ as eigenvalues. We denote with Λ_0^+ (or Λ_0^-) the positive (resp. negative) eigenspace. Λ_0^+ (resp. Λ_0^-) is the set of the points (x, ξ) such that $e^{-tY_0}(x, \xi) \to 0$ when $t \to +\infty$ (resp. $t \to -\infty$). Moreover $\Lambda_0^\pm$ are Lagrangian subspaces of $T^*\mathbb{R}^n$ given by $\xi_j = \pm\sqrt{\mu_j} x_j$. Then there exists two Lagrangian submanifolds $\Lambda^\pm$ tangent to $\Lambda_0^\pm$ in $(0,0)$ that are caracterized as the set of points (x, ξ) such that $\phi^t(x, \xi) \to (0,0)$ when $t \to \pm\infty$. Moreover there exists a neighborhood U of $(0,0)$ such that we can parametrize Λ^+ as the set of points $(x, \psi_1(x), \dots, \psi_n(x))$ with $\psi_i \in C^\infty(u)$ and such that

$$\frac{\partial \psi_i}{\partial x_j} = \frac{\partial \psi_j}{\partial x_i}$$

(because Λ^+ is Lagrangian). Then there exists a function $\varphi \in C^\infty(U)$ such that

$$\begin{cases} \frac{\partial \varphi}{\partial x_i}(x) = \psi_i(x) \\ \varphi(0) = 0 \end{cases}$$

and we get also

$$\varphi(x) = \varphi_0(x) + O(|x|^3)$$

because $T_{(0,0)}\Lambda^+ = \Lambda_0^+$. The equation (2.2.8) is equivalent to the statement $\Lambda^+ \subset q^{-1}(0)$. $\square$

Proposition 2.2.2 ([Hel88])**.** *Lex X be a C^∞ real vector field defined in a neighborhood of 0. Suppose that its linear part is given by:*

$$X_0 = \sum_{i=1}^n \nu_i x_i \partial_{x_i}$$

with $\nu_i > 0$. Let $b \in C^\infty$ a function such that $b(0) = 0$. Then for each function $g \in C^\infty$ such that $g(0) = 0$ and for each constant $\gamma \in \mathbb{R}$, there exists a unique function $f \in C^\infty$ defined in a neighborhood U of 0 such that

$$\begin{cases} (X + b)f = g \\ f(0) = \gamma \end{cases}$$

in U.

Proof. We can choose new coordinates y such that

$$y = x + O(|x|^2)$$

and

$$X = \sum_{i=1}^{n} \nu_i y_i \partial_{y_i}$$

In the new coordinates the problem becomes

$$\begin{cases} \left(\sum_{i=1}^{n} \nu_i y_i \partial_{y_i} + b(y) \right) f = g \\ \\ f(0) = \gamma \end{cases}$$

We reduce to $\gamma = 0$. Let $(t, y) \to \phi^t(y)$ the flow associated to X. Then

$$\phi^t(y) = (e^{\nu_j t} y_j)_{j=1,\dots,n}$$

Taking the norm, we get the estimate

$$|\phi^t(y)| \leq C e^{-\min_j \nu_j |t|} |y|$$

for $t \in]-\infty, 0]$. The solution is given by

$$f(y) = \int_{-\infty}^{0} g(\phi^t(y)) \exp\Big(- \int_t^0 b(\phi^s(y))\, ds \Big)\, dt$$

If $|g(y)| \leq C_N |y|^N$ then we have

$$|g(\phi^t(y))| \leq C_N C^N e^{-N \min_j \nu_j |t|} |y|^N$$
$$\left| - \int_t^0 b(\phi^s(y)) ds \right| \leq C_0 |t| |y|$$

Using these inequalities, we have

$$\left| g(\phi^t(y)) \exp\Big(- \int_t^0 b(\phi^s(y))\, ds \Big) \right| \leq C_N C^N |y|^N e^{(C_0 |y| - N \min_j \nu_j)|t|}$$

We assume $|y| \leq \varepsilon_0$ and we choose $N > \frac{C_0 \varepsilon_0}{\min_j \nu_j} + 1$. We get that

$$|f(y)| \leq \widetilde{C}_N |y|^N$$

We can apply the same argument to the derivative of f. □

Theorem 2.2.3 ([Hel88]). *Under the hypothesis (H1),(H2) and (H3), we can find a positive function $\varphi \in C^\infty(\mathbb{R}^n)$, a formal series:*

$$E(\varepsilon) \sim \sum_{j=0}^{\infty} \varepsilon^j E_j$$

where $E_0 = \min V = 0$, E_1 is the first eigenvalue of the associate harmonic oscillator and a formal symbol defined in a neighborhood of 0

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

and such that the following estimate holds in a neighborhood of 0*:*

$$(H(\varepsilon) - E(\varepsilon))(a(x,\varepsilon)e^{-\varphi(x)/\varepsilon}) = O(\varepsilon^\infty) \cdot e^{-\varphi(x)/\varepsilon} \tag{2.2.10}$$

Moreover

$$a(0,\varepsilon) = (2\pi)^{-n/4}$$

Proof. We formally insert $\psi = ae^{-\varphi/\varepsilon}$ in (2.2.10) and expand in powers of ε. We get

$$\sum_j \frac{\varepsilon^{j+2}}{2}\Delta a_j e^{-\varphi/\varepsilon} + \sum_j \varepsilon^{j+1}\nabla a_j \nabla\varphi e^{-\varphi/\varepsilon} + \sum_j V a_j e^{-\varphi/\varepsilon} - \sum_{i,j} \varepsilon^{i+j} E_j a_i e^{-\varphi/\varepsilon}$$
$$+ \sum_j \frac{\varepsilon^{j+1}}{2} a_j \Delta\varphi e^{-\varphi/\varepsilon} - \sum_j \varepsilon^j a_j |\nabla\varphi|^2 e^{-\varphi/\varepsilon}$$

Now the coefficient of ε^0 is equal to 0 if we have

$$\Big(-\frac{1}{2}|\nabla\varphi|^2 + (V - E_0)\Big)a_0 = 0$$

and from Proposition (2.2.1) we get the existence of a unique positive function φ solving the eikonal equation.
Then we look at the coefficient of ε^1 that is

$$2\nabla\varphi \cdot \nabla a_0 + (\Delta\varphi - 2E_1)a_0 = 0$$

with the initial condition $a_0(0) = (2\pi)^{-n/4}$, i.e. a transport equation as in Proposition (2.2.2) with $f = a_0$, $\gamma = (2\pi)^{-n/4}$, $g = 0$, and $b = \Delta\varphi - E_1$, if $b(0) = 0$. This last condition with (2.2.9) defines E_1:

$$E_1 = \frac{1}{2}\Delta\varphi(0) = \sum_{j=1}^{n} \sqrt{\mu_j}$$

The coefficient for ε^2 is

$$2\nabla\varphi \cdot \nabla a_1 + (\Delta\varphi - 2E_1)a_1 = -\Delta a_0 + 2E_2 a_0$$

with the initial condition $a_1(0) = 0$. We can apply again Proposition (2.2.2) with $f = a_1, \gamma = 0, b = \Delta\varphi - E_1$ and $g = -\Delta a_0 + E_2 a_0$, if $g(0) = 0$, that is

$$-\Delta a_0(0) + 2E_2 a_0(0) = 0$$

i.e.

$$E_2 = \frac{1}{2}\frac{\Delta a_0(0)}{a_0(0)}$$

(because $a_0(0) \neq 0$) and we can proceed in the same way for the other coefficients. □

2.2.2 Near a maximum of the potential

We will work on $\mathbb{T}^n$. We look for approxiamte solutions of the form

$$\psi(x) = a(x,\varepsilon)e^{\frac{i}{\varepsilon}\varphi(x)}$$

(Bloch wave form) with $a(x,\varepsilon) \sim \sum_k \varepsilon^k a_k(x)$, for the stationary Schrödinger equation

$$-\frac{\varepsilon^2}{2}\Delta\psi + (V - E)\psi = 0$$

In other words we are trying to construct a quasimode near the maximum of the potential. We make the following assumptions on the potential V:

(A1) $V'(0) = 0$

(A2) $V''(0) < 0$

Theorem 2.2.4. *Under the hypothesis (A1) and (A2) we can find a Lipschitz function $\varphi \in C^0(\mathbb{T}^n)$, a formal series:*

$$E(\varepsilon) \sim \sum_{j=0}^{\infty} \varepsilon^j E_j$$

where $E_0 = \max V$, $E_1 = 0$ and a formal symbol defined in a neighborhood of 0

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

and such that the following estimate holds in a neighborhood of 0*:*

$$\|(H(\varepsilon) - E(\varepsilon))(a(x,\varepsilon)e^{\frac{i}{\varepsilon}\varphi(x)})\|_{L^2} = O(\varepsilon^3) \tag{2.2.11}$$

Proof. Proceeding in the same way as in the previous theorem, we get

$$\left(-\frac{\varepsilon^2}{2}\Delta a - i\varepsilon\nabla a\cdot\nabla\varphi - \frac{i\varepsilon}{2}a\Delta\varphi + \frac{1}{2}a|\nabla\varphi|^2 + (V-E)a\right)e^{\frac{i}{\varepsilon}\varphi} = 0$$

The order 0 is given by the Hamilton-Jacobi equation

$$\left(\frac{1}{2}|\nabla\varphi|^2 + (V-E_0)\right)a_0 = 0$$

If we choose $E_0 = \max V$ then we know that there exist a (weak) Lipschitz solution $\varphi(x)$ defined on $\mathbb{T}^n$, that is C^3 in a neighborhood of 0.
If we look at the first order, we have

$$\left(\frac{1}{2}|\nabla\varphi|^2 + (V-E_0)\right)a_1 + E_1a_0 - i\left(\nabla a_0\cdot\nabla\varphi + \frac{1}{2}a_0\Delta\varphi\right) = 0$$

and we need to impose

$$\begin{cases} E_1 = 0 \\ \nabla a_0\cdot\nabla\varphi + \frac{1}{2}a_0\Delta\varphi = \operatorname{div}(a_0^2\nabla\varphi) = 0 \end{cases}$$

The second equation admits a (weak, in the sense of measure) solution a_0, as in [Eva07].
The second order is given by

$$\begin{aligned}\left(\frac{1}{2}|\nabla\varphi|^2 + (V-E_0)\right)a_2 + E_1a_1 - E_2a_0 - \frac{1}{2}\Delta a_0 - i\left(\nabla a_1\cdot\nabla\varphi + \frac{1}{2}a_1\Delta\varphi\right) \\ = -i\left(\nabla a_1\cdot\nabla\varphi + \frac{1}{2}a_1\Delta\varphi\right) - \left(\frac{1}{2}\Delta a_0 + E_2a_0\right) = 0\end{aligned}$$

and we can choose

$$E_2 = -\frac{1}{2}\frac{\Delta a_0(0)}{a_0(0)}$$

(we suppose here $a_0(0)\neq 0$). □

2.2.3 Another WKB approximation near the maximum

Now we try an alternative WKB approximation to get a result that will be useful in the following. As before we choose

$$\psi(x,\varepsilon) = a(x,\varepsilon)e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x)}$$

but we look for the following expansions

$$\begin{cases} a(x,\varepsilon) \sim \sum_k (\mathrm{i}\varepsilon)^k a_k(x) \\ E(\varepsilon) \sim \sum_k (\mathrm{i}\varepsilon)^k E_k \end{cases}$$

A similar construction can be found in [Laz93].

Theorem 2.2.5. *Under the hypothesis (A1) and (A2) we can find a Lipschitz function* $\varphi \in C^0(\mathbb{T}^n)$*, a formal series:*

$$E(\varepsilon) \sim \sum_{k=0}^{\infty} (\mathrm{i}\varepsilon)^k E_k$$

where $E_0 = \max V$*,* $E_1 = 0$ *and a formal symbol defined in a neighborhood of* 0

$$a(x,\varepsilon) \sim \sum_{k=0}^{\infty} (\mathrm{i}\varepsilon)^k a_k(x)$$

and such that the following estimate holds in a neighborhood of 0*:*

$$\|(H(\varepsilon) - E(\varepsilon))(a(x,\varepsilon)e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x)})\|_{L^2} = O(\varepsilon^3) \tag{2.2.12}$$

Proof. Proceeding in the usual way, we get

$$\left(-\frac{\varepsilon^2}{2}\Delta a - \mathrm{i}\varepsilon \nabla a \cdot \nabla\varphi - \frac{\mathrm{i}\varepsilon}{2} a\Delta\varphi + \frac{1}{2}a|\nabla\varphi|^2 + (V-E)a \right) e^{\frac{\mathrm{i}}{\varepsilon}\varphi} = 0$$

The order 0 is given by the Hamilton-Jacobi equation

$$\left(\frac{1}{2}|\nabla\varphi|^2 + (V - E_0)\right) a_0 = 0$$

If we choose $E_0 = \max V$ then we know that there exist a (weak) Lipschitz solution $\varphi(x)$ defined on $\mathbb{T}^n$, that is C^3 in a neighborhood of 0.
If we look at the first order, we have

$$\mathrm{i}\left(\frac{1}{2}|\nabla\varphi|^2 + (V - E_0)\right) a_1 + \mathrm{i}E_1 a_0 - \mathrm{i}\left(\nabla a_0 \cdot \nabla\varphi + \frac{1}{2}a_0\Delta\varphi\right) = 0$$

and again we need to impose

$$\begin{cases} E_1 = 0 \\ \nabla a_0 \cdot \nabla\varphi + \frac{1}{2}a_0\Delta\varphi = \operatorname{div}(a_0^2\nabla\varphi) = 0 \end{cases}$$

The second equation admits a (weak, in the sense of measure) solution a_0, as in [Eva07].

The second order is given by

$$-\left(\frac{1}{2}|\nabla\varphi|^2+(V-E_0)\right)a_2+E_1a_1+E_2a_0-\frac{1}{2}\Delta a_0-\mathrm{i}\left(\nabla a_1\cdot\nabla\varphi+\frac{1}{2}a_1\Delta\varphi\right)$$
$$=-\mathrm{i}\left(\nabla a_1\cdot\nabla\varphi+\frac{1}{2}a_1\Delta\varphi\right)-\left(\frac{1}{2}\Delta a_0-E_2a_0\right)=0$$

and we can choose

$$E_2=+\frac{1}{2}\frac{\Delta a_0(0)}{a_0(0)}$$

(we suppose here $a_0(0)\neq 0$). □

We constructed a, φ and E in this way because now we get the following Theorem.

Theorem 2.2.6. *The function $\bar{H}_\varepsilon(P)$ for $P=0$ in (2.1.14) concides with the real part of the function $E(\varepsilon)$ constructed in Theorem 2.2.5 up to second order terms. That means*

$$|\bar{H}_\varepsilon(0)-\operatorname{Re}E(\varepsilon)|=O(\varepsilon^3)$$

Proof. In the previous theorem we constructed the function $E(\varepsilon)$ as

$$E(\varepsilon)=\max V+\frac{\varepsilon^2}{2}\frac{\Delta a_0(0)}{a(0)}+O(\varepsilon^3)$$

We recall here some definitions that the reader can find in [Eva07] and also in the previous chapter. Define $w(x)$, $v(x)$ and $E(0,\varepsilon)$ as the solution of

$$\begin{cases}-\dfrac{\varepsilon^2}{2}\Delta w-Vw=E(0,\varepsilon)w\\ -\dfrac{\varepsilon}{2}\Delta v+\dfrac{|\nabla v|^2}{2}+V=\max V\end{cases}$$

In particular

$$\bar{H}_\varepsilon(0)=-E(0,\varepsilon)=\max V+\frac{\varepsilon^2}{2}\frac{\Delta w}{w}$$

and computing the Taylor series around $\varepsilon=0$ we get

$$\bar{H}_\varepsilon(0)=\bar{H}_\varepsilon(0)_{|\varepsilon=0}+\frac{d}{d\varepsilon}\bar{H}_\varepsilon(0)_{|\varepsilon=0}\varepsilon+\frac{d^2}{d\varepsilon^2}\bar{H}_\varepsilon(0)_{|\varepsilon=0}\varepsilon^2+O(\varepsilon^3)$$
$$=\max V+\frac{\varepsilon^2}{2}\frac{\Delta w_0(0)}{w_0(0)}+O(\varepsilon^3)$$

where we assume that $w \sim \sum_k \varepsilon^k w_k$ and $v \sim \sum_k \varepsilon^k v_k$ and w_0, v_0 solve

$$\begin{cases} \frac{1}{2} w_0 \Delta v_0 + \nabla w_0 \cdot \nabla v_0 = 0 \\ \frac{|\nabla v_0|^2}{2} + V = \max V \end{cases}$$

and so we have $w_0 = a_0$ and $v_0 = \varphi$. $\square$

Chapter 3

WKB approximation of the Schrödinger evolutive equation

3.1 FIO and WKB

In the time independent WKB approximation the starting point is one the following ansatzs

$$\psi(x) = e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x)}A(\varepsilon, x)$$
$$\psi(x) = \int_{\Theta} e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x,\theta)}A(\varepsilon, x, \theta)d\theta$$

where $\Theta = \mathbb{R}^N$ (the set of frequencies), φ is a real phase and the amplitude A admits the following expansion in powers of ε: $A(\varepsilon, x, \theta) \sim \sum \varepsilon^j A_j(x, \theta)$. Let $K(\varepsilon, t, x, y)$ the propagator of the time dependent Schrödinger operator, that is the Schwartz kernel of the unitary operator $U_H(t)$. K satisfies

$$\begin{cases} \mathrm{i}\varepsilon\dfrac{\partial}{\partial t}K(\varepsilon, t, x, y) = HK(\varepsilon, 0, x, y) \\ K(\varepsilon, t, x, y) = \delta(x-y) \end{cases} \tag{3.1.1}$$

We will look for solutions of the form

$$K(\varepsilon, t, x, y) = \int_{\Theta} e^{\frac{\mathrm{i}}{\varepsilon}\varphi(t,x,\theta,y)}A(\varepsilon, x, \theta, y)d\theta \tag{3.1.2}$$

and we assume that the quantum Hamiltonian is of the following type

$$H = -\varepsilon^2\Delta + V \tag{3.1.3}$$

where the potential V is assumed to be smooth and satisfies the estimate

$$|\partial_x^\alpha V(x)| \leq C_\alpha \left(1 + |x|^2\right)^{\frac{1}{2}(2-|\alpha|)_+} \tag{3.1.4}$$

for every α multindex and for every $x \in \mathbb{R}^n$. We make for K the following ansatz

$$K(\varepsilon, t, x, y) = (2\pi\varepsilon)^{-n} \int_{\Theta} e^{\frac{\mathrm{i}}{\varepsilon}(S(t,x,\eta)-\langle y,\eta\rangle)} \left(\sum_{j\geq 0} \varepsilon^j A_j(t, x, \eta) \right) d\eta$$

with the initial conditions at $t = 0$

$$S(0, x, \eta) = \langle x, \eta \rangle$$
$$A_0(0, x, \eta) = 1$$
$$A_j(0, x, \eta) = 0, \text{ for } j \geq 1$$

Now starting from (3.1.1) and computing the expansion in ε, we get the following equation for S

$$\partial_t S(t, x, \eta) + H(x, \partial_x S(t, x, \eta)) = 0 \tag{3.1.5}$$

that is an Hamilton-Jacobi equation for S, and the sequence of transport equations for A_j

$$\mathrm{i}\partial_t A_0(t, x, \eta) = \mathcal{L}(x, \eta, D_x) A_0(t, x, \eta) \tag{3.1.6}$$
$$\mathrm{i}\partial_t A_j(t, x, \eta) = \mathcal{L}(x, \eta, D_x) A_j(t, x, \eta) + F_j(A_0, \ldots, A_j) \tag{3.1.7}$$

where $\mathcal{L}(x, \eta, D_x)$ represents the following differential operator

$$\mathcal{L}(x, \eta, D_x)B = \partial_p H \cdot D_x B + (2\mathrm{i})^{-1} \left[\mathrm{tr} \left(\partial^2_{p,p} H(x, \partial_x S) \cdot \partial^2_{x,x} + \partial^2_{x,p} H(x, \partial_x S) \right) \right] B$$

and the F_j's are polynomial in a finite number of derivatives of $A_0, \ldots, A_j$, with uniformily bounded coefficients.

Theorem 3.1.1. *There exists $T > 0$ small enough such that*

(i) The HJ equation (3.1.5) has a unique solution $S(t, x, \eta)$. Moreover one has

$$\Phi_H^{-t}(x, \partial_x S(t, x, \eta)) = (\partial_\eta S(t, x, \eta), \eta)$$

and S satisfies the following estimate ($z = (x, \eta)$):

$$|\partial_z^\gamma S(t, z)| \leq C(1 + |z|^2)^{\frac{1}{2}(2-|\gamma|)_+}$$

(ii) The transport equations (3.1.6) and (3.1.7) admit by induction, a sequence of unique solutions $A_j(t, x, \eta) \in C^\infty([-T, T] \times Z)$, that satisfy

$$\left| \partial_t^k \partial_z^\gamma A_j(t, z) \right| \leq C$$

for all $(t, z) \in [-T, T] \times Z$.

(iii) Introducing the FIO

$$U_{H,N}(t)\psi(x) = (2\pi\varepsilon)^{-n}\int_Z e^{\frac{\mathrm{i}}{\varepsilon}(S(t,x,\eta)-\langle y,\eta\rangle)}\left(\sum_{0\le j\le N}\varepsilon^j A_j(t,x,\eta)\right)\psi(y)dyd\eta \tag{3.1.8}$$

we have the following remainder

$$\sup_{|t|\le T}\|U_H(t)-U_{H,N}(t)\|_{L^2} = O(\varepsilon^N) \tag{3.1.9}$$

Proof. Following [Rob87] and [HR83]. The Hamilton-Jacobi and transport equations can be solved using standard methods (integration along the classical flow): thus the time $T>0$ is determined by the presence of caustics. For the estimates:

$$(\mathrm{i}\varepsilon\partial_t - H)U_{H,N}(t) = R_N(\varepsilon;t) \tag{3.1.10}$$

where $R_N(\varepsilon;t)$ is the Fourier Integral Operator defined by

$$R_N(\varepsilon;t)\varphi(x) = (2\pi\varepsilon)^{-n}\int_Z r_N(\varepsilon;t,x,\eta)e^{\frac{\mathrm{i}}{\varepsilon}(S(t,x,\eta)-\langle x,\eta\rangle)}dxd\eta$$

where $\varepsilon^{-N-1}r_N(t,x,\cdot)$ is of order $\mathcal{O}(0)$ for $t\in[-T,T]$ and $\varepsilon\in]0,\varepsilon_0]$. This implies that there exists a constant $C>0$ such that

$$\|R_N(\varepsilon;t)\|\le C\varepsilon^{N+1}$$

for all $t\in[-T,T]$ and all $\varepsilon\in]0,\varepsilon_0]$. $\square$

Group property

We want to construct approximations for $U_H(t)$ for every time t. We can do this using the group property of the operator. Fix $T_1\in]0,T/2[$, consider $t\in]kT_1,(k+1)T_1[$ and assume $k\ge 1$. Then

$$U_H(t) = U_H(t-kT_1)\cdot U_H(T_1)^k$$

and we can approximate it by

$$V_{H,N}(t) = U_{H,N}(t-kT_1)\cdot U_{H,N}(T_1)^k$$

From the estimate (3.1.9), we get the following estimate

$$\sup_{kT_1\le t\le(k+1)T_1}\|U_H(t)-V_{H,N}(t)\|_{L^2} = O(\varepsilon^N)$$

$V_{H,N}(t)$ is a FIO: applying the product rule for FIO, we get $V_{H,N}(t) = \mathcal{I}(\phi, B, \varepsilon)$ with

$$\phi(t,x,\theta,y) = S(t-kT_1, x, \eta_{k+1}) - \langle y_{k+1}, \eta_{k+1}\rangle + \sum_{1\le j\le k} S(T_1, y_{j+1}, \eta_j) - \langle y_j, \eta_j\rangle$$

$$y = y_1, \;\; \theta = (\eta_1, y_2, \eta_2, \dots, y_{k+1}, \eta_{k+1}) \in (\mathbb{R}^n)^{2k+1}$$

$$B(\varepsilon; t, x, \theta, y) = A^{(N)}(\varepsilon; t-kT_1, x, \eta_{k+1}) \prod_{j=1}^{j=k} A^{(N)}(\varepsilon; T_1, y_{j+1}, \eta_j)$$

where

$$A^{(N)}(\varepsilon; t, x, \eta) = \sum_{0\le j\le N} \varepsilon^j A_j(t,x,\eta)$$

A similar result can be found in [GZ10]: in their work the authors are able to construct a multivalued WKB approximation of the Schrödinger evolution operator.
There is another interesting possible connection between the construction of the FIO using the group property and the so called Symplectic Homogenization of Viterbo in [Vit08], since the phase of the FIO is constructed precisely using the composition rule for generating functions. In Viterbo's notations

$$F_k(x,p;\xi) = \sum_{j=1}^{k} S(t_j, \xi_j, p_j) + Q_k(x,p;\xi) - \langle p, x\rangle$$

is the generating function of the k-th composition of the flow. More precisely, Viterbo consider the following function.

Definition 3.1.2. *We define*

$$h_k(p) := c(\mu_x, F_{k,p})$$

where $F_{k,p} = F_k(x,p;\xi)$.

The detailed definition of $c(\mu_x, F_{k,p}) = c(\mu_x \otimes 1(\xi), F_k(p))$ arises from the min-max theory in the cohomological setting, see [Vit08]. The author is then able to prove that the sequence $\{h_k\}_{k\in\mathbb{N}}$ c-converges to a function $h_\infty(p)$ (the c-convergence is a weak convergence for the flows). It turns out that h_∞ coincides with the α Mather function (or equivalently the homogenization of the Hamiltonian h).

Remark 3.1.3 The definition of h_k is based essentially on the search for a critical value for η fixed and x and the parameters ξ are free to vary. To the 0-dimensional cohomology generator (the cohomology of the points), i.e. $1(\xi)$ in our case, corresponds the minimum, while to the volume form μ_x correspond a maximum or a saddle point (depending on the compactness of the manifold). For this we can conjecture that the critical value $c(\mu_x \otimes 1(\xi), F_k)$ can be written as an inf max. More precisely, this does work whenever F_k is positive definite in the auxiliary parameters ξ, one would have

$$c(\mu_x \otimes 1(\xi), F_k) = \inf_{\xi\in\mathbb{R}^{2(k-1)}} \max_{x\in\mathbb{T}^n} F_k(x, p; \xi) \tag{3.1.11}$$

It is interesting to notice that if (3.1.11) holds true, then one must have

$$h_\infty(p) = \lim_{k\to\infty} \inf_{\xi\in\mathbb{R}^{2(k-1)}} \max_{x\in\mathbb{T}^n} F_k(x, p; \xi)$$

and, since h_∞ coincides with the homogeneized Hamiltonian, we would have

$$\lim_{k\to\infty} \inf_{\xi\in\mathbb{R}^{2(k-1)}} \max_{x\in\mathbb{T}^n} F_k(x, p; \xi) = \inf_{f\in C^1(\mathbb{T}^n)} \max_{x\in\mathbb{T}^n} H(x, \nabla f + p) = \bar{H}(p)$$

To conclude this remark, note that the limit $k \to \infty$ for the numbers of parameters, corresponds to the limit $t \to \infty$ for the time of the phase of the FIO: this would mean that, for large times, the phase c-converge to $\bar{H}(p)$.

3.2 Madelung approach

In the following we will make the following hypothesis on the Hamiltonian:

(i) $H : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$, $H(x,p) = \frac{p^2}{2} + V(x)$ (we will consider only mechanical Hamiltonians);

(ii) $V(x)$ has only non degenerate maxima $(x_i)_{1\le i\le m}$;

(iii) there exists only one $x_I \in \{x_i | 1 \le i \le m\}$ that minimizes $\sum_{j=1}^m \sqrt{k_j(x_i)}$ where $-k_j(x_i)$ is the j-th eigenvalue of the Hessian of V at the point x_i.

Without loss of generality we will suppose that $x_I = 0$ (it will be clear in the following chapters why we have made these hypothesis). We will look for an approximate solution of the time dependent Schrödinger equation on $\mathbb{T}^d$

$$\begin{cases} i\varepsilon\partial_t\psi^t = H\psi^t \\ \psi(0,x) = \psi_{(0,0)} \end{cases} \tag{3.2.1}$$

where $\psi_{(0,0)}$ is a (Gaussian) coherent state centered in $(0,0) \in \mathbb{T}^d \times \mathbb{R}^d$, where $H = -\frac{\varepsilon^2}{2}\Delta + V$, of the form

$$\psi(t,x) = A(t,x)e^{\frac{i}{\varepsilon}S(t,x)}$$

and we will use WKB approximation both in the amplitude and in the phase

$$A(t,x) \sim \sum_k \varepsilon^k A_k(t,x) \quad S(t,x) \sim \sum_l \varepsilon^l S_l(t,x)$$

We will find a series of partial differential equation and we will compute the remainder of the approximation of order 2. The problem is to find an (a priori) estimate for this remainder.

Some Computations

Using the WKB approximation

$$\psi(t,x) = \Big(\sum_k \varepsilon^k A_k(t,x)\Big)e^{\frac{i}{\varepsilon}\sum_l \varepsilon^l S_l(t,x)}$$

we transform the Schrödinger equation into

$$\Big(\sum_{k,l} A_k \partial_t S_l + \frac{1}{2}\sum_{k,l,m} \varepsilon^{k+l+m} A_k(\partial_x S_l)(\partial_x S_m) + \sum_k \varepsilon^k A_k V - \frac{1}{2}\sum_k \varepsilon^{k+2}\partial_{xx}A_k\Big) \tag{3.2.2}$$

$$+i\varepsilon\Big(\sum_k \varepsilon^k \partial_t A_k + \sum_{k,l} \varepsilon^{k+l}\Big(\partial_x A_k \partial_x S_l + \frac{1}{2}A_k \partial_{xx} S_l\Big)\Big) = 0 \tag{3.2.3}$$

so we get the following series of sistem of PDEs

$$\begin{cases} \sum_{k,l} A_k \partial_t S_l + \frac{1}{2}\sum_{k,l,m} \varepsilon^{k+l+m} A_k(\partial_x S_l)(\partial_x S_m) + \sum_k \varepsilon^k A_k V - \frac{1}{2}\sum_k \varepsilon^{k+2}\partial_{xx}A_k = 0 \\ \sum_k \varepsilon^k \partial_t A_k + \sum_{k,l} \varepsilon^{k+l}\Big(\partial_x A_k \partial_x S_l + \frac{1}{2}A_k \partial_{xx} S_l\Big) = 0 \end{cases}$$

Now, looking at order $0, 1$ and 2, we get

$$\varepsilon^0 : \begin{cases} \partial_t S_0 + \frac{1}{2}(\partial_x S_0)^2 + V = 0 \\ \partial_t A_0 + \partial_x A_0 \partial_x S_0 + \frac{1}{2}A_0 \partial_{xx} S_0 = 0 \end{cases}$$

$$\varepsilon^1 : \begin{cases} \partial_t S_1 + (\partial_x S_0)(\partial_x S_1) = 0 \\ \partial_t A_1 + \partial_x A_1 \partial_x S_0 + \frac{1}{2}A_1 \partial_{xx} S_0 = -(\partial_x A_0 \partial_x S_1 + \frac{1}{2}A_0 \partial_{xx} S_1) \end{cases}$$

$$\varepsilon^2: \begin{cases} \partial_t S_2 + (\partial_x S_0)(\partial_x S_2) = \frac{1}{2}\frac{\partial_{xx} A_0}{A_0} - \frac{1}{2}(\partial_x S_1)^2 \\ \partial_t A_2 + \partial_x A_2 \partial_x S_0 + \frac{1}{2} A_2 \partial_{xx} S_0 = \\ = -(\partial_x A_0 \partial_x S_2 + \frac{1}{2} A_0 \partial_{xx} S_2 + \partial_x A_1 \partial_x S_1 + \frac{1}{2} A_1 \partial_{xx} S_1) \end{cases}$$

Note that order 0 can be rewritten as

$$\begin{cases} \partial_t S_0 + \frac{1}{2}(\partial_x S_0)^2 + V = 0 \\ \partial_t A_0^2 + \partial_x (A_0^2 \partial_x S_0) = 0 \end{cases}$$

and so the first equation is an Hamilton-Jacobi PDE and the second is a continuity equation. Looking at the first and second order equations we have a transport equation and something similar to a continuity equation.

Reducing the equations

In this section we will look closer to the equations and we will try to simplify them. Take the first order system

$$\varepsilon^1: \begin{cases} \partial_t S_1 + (\partial_x S_0)(\partial_x S_1) = 0 \\ \partial_t A_1 + \partial_x A_1 \partial_x S_0 + \frac{1}{2} A_1 \partial_{xx} S_0 = -(\partial_x A_0 \partial_x S_1 + \frac{1}{2} A_0 \partial_{xx} S_1) \end{cases}$$

A possible solution of the first equation is $S_1(t,x) = c \in \mathbb{R}$. But if we look at the initial datum on the phase $S(0,x) = 0$, we have that $S_1(t,x) = 0$. In particular the systems of equations become

$$\varepsilon^0: \begin{cases} \partial_t S_0 + \frac{1}{2}(\partial_x S_0)^2 + V = 0 \\ \partial_t A_0^2 + \partial_x (A_0^2 \partial_x S_0) = 0 \end{cases}$$

$$\varepsilon^1: \begin{cases} S_1(t,x) = 0 \\ \partial_t A_1^2 + \partial_x (A_1^2 \partial_x S_0) = 0 \end{cases}$$

$$\varepsilon^2: \begin{cases} \partial_t S_2 + (\partial_x S_0)(\partial_x S_2) = \frac{1}{2}\frac{\partial_{xx} A_0}{A_0} \\ \partial_t A_2 + \partial_x A_2 \partial_x S_0 + \frac{1}{2} A_2 \partial_{xx} S_0 = -(\partial_x A_0 \partial_x S_2 + \frac{1}{2} A_0 \partial_{xx} S_2) \end{cases}$$

Now the first system is again Hamilton-Jacobi + Continuity equation; the second system has only the (same!) Continuity equation (but the solution could be different depending on a different initial datum for A_1) while the third system is given by a Transport equation and something similar to a Continuity equation.

The remainder

Suppose that we have found the solutions up to the second order approximation: we build the wave function

$$\psi(t,x) = (A_0 + \varepsilon A_1 + \varepsilon^2 A_2)e^{\frac{i}{\varepsilon}(S_0+\varepsilon S_1+\varepsilon^2 S_2)}$$

and we put it into the Schrödinger equation and compute the remainder $R(t,x)$:

$$i\varepsilon\psi(t,x) - H\psi(t,x) = R(t,x)$$

The real part is given by

$$\begin{aligned}\operatorname{Re} R(t,x) = {} & \varepsilon^3\Big[\frac{1}{2}\frac{A_1}{A_0}\partial_{xx}A_0 - \frac{1}{2}\partial_{xx}A_1 + A_0(\partial_x S_1)(\partial_x S_2)\Big] \\ & + \varepsilon^4\Big[\frac{1}{2}\frac{A_2}{A_0}\partial_{xx}A_0 - \frac{1}{2}\partial_{xx}A_2 + A_0(\partial_x S_2)^2 + A_1(\partial_x S_1)(\partial_x S_2)\Big] \\ & + \varepsilon^5\Big[A_1(\partial_x S_2) + A_2(\partial_x S_1)(\partial_x S_2)\Big] \\ & + \varepsilon^6\Big[\frac{1}{2}(\partial_x S_2)^2\Big]\end{aligned}$$

while the imaginary part is

$$\begin{aligned}\operatorname{Im} R(t,x) = {} & \varepsilon^3\Big[\frac{1}{2A_1}\partial_x(A_1^2\partial_x S_2) + \frac{1}{2A_2}\partial_x(A_2^2\partial_x S_1)\Big] \\ & + \varepsilon^4\Big[\frac{1}{2A_2}\partial_x(A_2^2\partial_x S_2)\Big]\end{aligned}$$

Knowing that $\partial_x S_1 = 0$ we can simplify the remainder:

$$\begin{aligned}\operatorname{Re} R(t,x) = {} & \varepsilon^3\Big[\frac{1}{2}\frac{A_1}{A_0}\partial_{xx}A_0 - \frac{1}{2}\partial_{xx}A_1\Big] \\ & + \varepsilon^4\Big[\frac{1}{2}\frac{A_2}{A_0}\partial_{xx}A_0 - \frac{1}{2}\partial_{xx}A_2 + A_0(\partial_x S_2)^2\Big] \\ & + \varepsilon^5\Big[A_1(\partial_x S_2)\Big] \\ & + \varepsilon^6\Big[\frac{1}{2}(\partial_x S_2)^2\Big]\end{aligned}$$

$$\begin{aligned}\operatorname{Im} R(t,x) = {} & \varepsilon^3\Big[\frac{1}{2A_1}\partial_x(A_1^2\partial_x S_2)\Big] \\ & + \varepsilon^4\Big[\frac{1}{2A_2}\partial_x(A_2^2\partial_x S_2)\Big]\end{aligned}$$

Using T.Paul Lemma we can estimate

$$\|R(t,x)\| \leq Ct\varepsilon^2 \sup_{s\in[0,t]} |T(s,x)|$$

where $T(t,x)$ is simply $R(t,x)$ where we have taken out the common factor ε^3. So the problem is to find an (a priori) estimate for

$$\sup_{s\in[0,t]} |T(t,x)| \leq \frac{1}{2}\sup_{s\in[0,t]}\Big|\frac{A_1\partial_{xx}A_0 - A_0\partial_{xx}A_1}{A_0} + \frac{\partial_x(A_1^2\partial_x S_2)}{A_1}\Big|$$

3.3 Other systems of PDEs

Madelung and Fokker-Planck

Instead of considering the "classical" system of PDEs

$$\begin{cases} \partial_t S + H(x,\nabla S) = \frac{\varepsilon^2}{2}\frac{\Delta A}{A} \\ \partial_t P + \operatorname{div}(P\nabla S) = 0 \end{cases}$$

(where $A = \sqrt{P}$), we want to study a new one given by

$$\begin{cases} \partial_t S + H(x,\nabla S) = \frac{\varepsilon^2}{2}\frac{\Delta A}{A} \\ \partial_t P + \operatorname{div}(P\nabla S) = \nu(\varepsilon)\Delta P \end{cases} \tag{3.3.1}$$

Again: $A = \sqrt{P}$ and $\nu(\varepsilon)$ is the viscosity constant (and we consider it as a function of ε). Note that this (toy?) model satisfy

$$\frac{d}{dt}\int_{\mathbb{T}^n} P(t,x)dx = -\int_{\mathbb{T}^n} \nabla\cdot(P\nabla S - \nu(\varepsilon)\nabla P)dx = 0$$

First of all we look for the existence of equilibrium points: so we need to find the solutions of the stationary system

$$\begin{cases} H(x,\nabla S) = E_\varepsilon + \frac{\varepsilon^2}{2}\frac{\Delta A}{A} \\ \operatorname{div}(P\nabla S) = \nu(\varepsilon)\Delta P \end{cases} \tag{3.3.2}$$

Definition 3.3.1. *We will say that $(S(x), P(x), E_\varepsilon)$ (where $x\in\mathbb{T}^n$) is an equilibrium point of (3.3.1) if it solves (3.3.2)*

We can state now the existence of an equilibrium point.

Proposition 3.3.2. *An equilibrium point for (3.3.1) is given by $(S_\varepsilon(x), e^{\frac{S_\varepsilon(x)}{\nu}}, E_\varepsilon)$ where $S_\varepsilon(x)$ is the unique (up to a constant) solution of*

$$\frac{1}{2}\left(1-\frac{\varepsilon^2}{4\nu^2}\right)|\nabla S(x)|^2 + V(x) = E_\varepsilon + \frac{\varepsilon^2}{4\nu}\Delta S(x) \tag{3.3.3}$$

and E_ε is the unique constant associated to S_ε.

Proof. If $P_\varepsilon(x) = e^{\frac{S_\varepsilon(x)}{\nu}}$ then

$$\nu(\varepsilon)\Delta P_\varepsilon = \nu(\varepsilon)\nabla\cdot(\nabla P_\varepsilon) = \nabla\cdot(e^{\frac{S_\varepsilon(x)}{\nu}}\nabla S_\varepsilon)$$
$$\nabla\cdot(P_\varepsilon\nabla S_\varepsilon) = \nabla\cdot(e^{\frac{S_\varepsilon(x)}{\nu}}\nabla S_\varepsilon)$$

so P_ε solves the Fokker-Planck stationary equation. Now computing

$$\begin{aligned}\frac{\varepsilon^2}{2}\frac{\Delta\sqrt{P_\varepsilon}}{\sqrt{P_\varepsilon}} &= \frac{\varepsilon^2}{2}e^{-\frac{S_\varepsilon}{2\nu}}\left(\frac{\Delta S_\varepsilon}{2\nu}e^{\frac{S_\varepsilon}{2\nu}} + \frac{|\nabla S_\varepsilon|^2}{4\nu^2}e^{\frac{S_\varepsilon}{2\nu}}\right)\\ &= \frac{1}{2}\frac{\varepsilon^2}{4\nu^2}|\nabla S_\varepsilon|^2 + \frac{\varepsilon^2}{4\nu}\Delta S_\varepsilon\end{aligned}$$

that inserted in the first equation gives (3.3.3). □

Hamilton-Jacobi and Fokker-Planck

Now we try to study a problem that seems simpler:

$$\begin{cases}\partial_t S + H(x,\nabla S) = 0\\ \partial_t P + \mathrm{div}(P\nabla S) = \nu\Delta P\end{cases} \tag{3.3.4}$$

Clearly an equilibrium of this system of equations is given by

$$\begin{cases}H(x,\nabla\widehat{S}) = E\\ \mathrm{div}(\widehat{P}\nabla\widehat{S}) = \nu\Delta\widehat{P}\end{cases}$$

and the second equation admits $\widehat{P}(x) = e^{\frac{\widehat{S}(x)}{\nu}}$ as a solution. Moreover, the functional

$$I(t) = \int P(t,x)\ln\frac{P(t,x)}{\widehat{P}(x)}dx$$

is a Lyapunov function for the Fokker-Planck equation (that means $\frac{d}{dt}I(t) \le 0$ and $\frac{d}{dt}I(t) = 0$ if and only if $P(t,x) = \widehat{P}(x)$). The Hamilton-Jacobi equation is unique up to a constant, so we have to choose this constant in order to have

$$\int_{\mathbb{T}^n}\widehat{P}(x)dx = 1$$

i.e. the equilibrium must be a probability on $\mathbb{T}^n$.

Example 3.3.3. We make an example: the free particle on $\mathbb{T}^1$. The equilibrium equations will be given by

$$\begin{cases} |\partial_x \widehat{S}(x)|^2 = 0 \\ \partial_{xx} \widehat{P}(x) = 0 \end{cases}$$

The second equation gives $\widehat{P}(x) = Ax + B$, but, because $\widehat{P}$ must be a probability

$$\int_0^1 Ax + B \, dx = 1$$

and we get $B = 1 - \frac{A}{2}$. Moreover $\widehat{P}(x) = e^{C/\nu}$ (must be a constant) so we must have $A = 0$ and we finally find $(\widehat{S}(x), \widehat{P}(x)) = (0, 1)$. In this situation we will have $\lim_{t\to\infty} \|S(t,x) - \widehat{S}(x)\|_\infty = \lim_{t\to\infty} \|S(t,x)\| = 0$ and $P(t,x) \overset{t\to\infty}{\to} 1$.

Going back to NLS equations

Now we try to get back to the equations that originates the systems that we have seen before.

Proposition 3.3.4. *(i) If the couple $(S(t,x), P(t,x))$ solves the system of PDEs (3.3.1), then $\psi(t,x) = \sqrt{P(t,x)}\, e^{\frac{i}{\varepsilon}S(t,x)}$ solves*

$$i\varepsilon \partial_t \psi = -\frac{\varepsilon^2}{2}\Delta\psi + V(x)\psi + \frac{i\varepsilon}{2}\nu \frac{\psi}{|\psi|^2}\Delta|\psi|^2 \tag{3.3.5}$$

(ii) If the couple $(S(t,x), P(t,x))$ solves (3.3.4), then $\psi(t,x) = \sqrt{P(t,x)}\, e^{\frac{i}{\varepsilon}S(t,x)}$ solves

$$i\varepsilon \partial_t \psi = -\frac{\varepsilon^2}{2}\Delta(\psi - |\psi|) + V(x)\psi + \frac{i\varepsilon}{2}\nu \frac{\psi}{|\psi|^2}\Delta|\psi|^2 \tag{3.3.6}$$

Chapter 4

Semiclassical limit and WKAM Theorem

In this chapter we present some known tools and few final elaborations useful to the results worked out in chapter 1. Here we will follow mainly [Sib04] and [AIPSM05].

4.1 Mather's Minimal Action

Consider the n-dimensional torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$. Denote with (x, v) the coordinates on $T\mathbb{T}^n = \mathbb{T}^n \times \mathbb{R}^n$. Let $L : \mathbb{S}^1 \times T\mathbb{T}^n \to \mathbb{R}$ of class C^2.

Definition 4.1.1. *The action of a curve C^1 $\gamma : [a, b] \to \mathbb{T}^n$ is defined as*

$$A(\gamma) := \int_a^b L(t, \gamma(t), \dot{\gamma}(t))dt$$

It is a well known fact that the curves that extremize the action functional solve Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial v}(t, \gamma(t), \dot{\gamma}(t)) = \frac{\partial L}{\partial x}(t, \gamma(t), \dot{\gamma}(t)) \tag{4.1.1}$$

for all $t \in [a, b]$. To solve equation (4.1.1) is equivalent to solve

$$\frac{\partial^2 L}{\partial v^2}(t, \gamma(t), \dot{\gamma}(t))\ddot{\gamma}(t) = \frac{\partial L}{\partial x}(t, \gamma(t), \dot{\gamma}(t)) - \frac{\partial^2 L}{\partial x \partial v}(t, \gamma(t), \dot{\gamma}(t))\dot{\gamma}(t) \tag{4.1.2}$$

and if the Lagrangian L satisfies Legendre condition

$$\det \frac{\partial^2 L}{\partial v^2} \neq 0$$

then it is possible to solve (4.1.2). Moreover it is well defined a vector field $X_L(t, x, v) = ((x, v), (v, X_L^\pi(t, x, v))$ over $T(T\mathbb{T}^n)$ such that the solutions of $\ddot{\gamma}(t) = X_L^\pi(t, x, v)$ are exactly the solutions of (4.1.1).

Definition 4.1.2. *The vector field X_L is called Euler-Lagrange vector field and its flow φ_L is the Euler-Lagrange flow.*

Remark 4.1.3 Even if L is only of class C^2, φ_L is in C^1.

Definition 4.1.4. *A convex Lagrangian is a C^2 function such that the following conditions hold:*

(i) restricted to every fiber $\{t\} \times T_x\mathbb{T}^n$, L is strictly convex; i.e.

$$\frac{\partial^2 L}{\partial v^2} > 0$$

for all $v \in \{t\} \times T_x\mathbb{T}^n$;

(ii) L has a superlinear growth (with respect to some Riemannian metric)

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

uniformly in x;

(iii) the Euler-Lagrange flow φ_L is complete; i.e. its solutions exist for all times.

Remark 4.1.5 A Lagrangian L is not uniquely determined by its flow φ_L. Indeed if L generates φ_L, then also every Lagrangian of the form

$$L_\eta(x,v) := L(x,v) - \eta_x(v)$$

where η is any closed 1-form on the torus $\mathbb{T}^n$, generates the same flow φ_L. If we consider the two actions $\int_\gamma L_\eta$ and $\int_\gamma L$, we can see that they differ for the term $\int_\gamma \eta$. Since η is a closed 1-form, using Stokes' Theorem we know that this integral does not depend on γ, but only on the initial and final points and so it is a constant. The two actions differ by a constant and so generate the same Euler-Lagrange flow φ_L. Moreover if L is convex, then the new Lagrangian L_η is also convex.

In the following we will consider only convex Lagrangian and we will not deal with orbits of Euler-Lagrangian flow, but rather with invariant probability measures.

Definition 4.1.6. *Let $\mathcal{M}_L$ be the set of φ_L-invariant probability measures. We define the action of $\mu \in \mathcal{M}_L$ as*

$$A(\mu) = \int L \, d\mu \quad \in \mathbb{R} \cup \{+\infty\}$$

For every $\mu \in \mathcal{M}_L$ we associate the linear functional

$$\begin{aligned} H^1(\mathbb{T}^n, \mathbb{R}) &\to \mathbb{R} \\ [\eta] &\mapsto \int \eta \, d\mu \end{aligned}$$

where we consider a 1-form ν as a function on $T\mathbb{T}^n$ that is linear on the fibers. By duality there exists a unique class $\rho(\mu) \in H^1(\mathbb{T}^n, \mathbb{R})$ such that

$$\int \eta \, d\mu = \langle [\eta] | \rho(\mu) \rangle \tag{4.1.3}$$

for all $[\eta] \in H^1(\mathbb{T}^n, \mathbb{R})$.

Definition 4.1.7. *The class $\rho(\mu) \in H_1(\mathbb{T}^n, \mathbb{R})$ defined by (4.1.3), is called the rotation vector of μ.*

Definition 4.1.8. *Let L be a convex Lagrangian. Then the function*

$$\begin{aligned} \alpha : H_1(\mathbb{T}^n, \mathbb{R}) &\to \mathbb{R} \\ h &\mapsto \min\{A(\mu) \,|\, \mu \in \mathcal{M}_L, \; \rho(\mu) = h\} \end{aligned}$$

is calles the minimal action of L. Every invariant measure $\mu \in \mathcal{M}_L$, i.e. with $A(\mu) = \alpha(\rho(\mu))$ realizing the minimum, is called minimal measure.

Proposition 4.1.9. *The minimal action $\alpha : H_1(\mathbb{T}^n, \mathbb{R}) \to \mathbb{R}$ is a convex, superlinear function.*

Proof. Let $h_1, h_2 \in H_1(\mathbb{T}^n, \mathbb{R})$ and $\lambda \in [0, 1]$. Choose minimal measures $\mu_1, \mu_2 \in \mathcal{M}_L$ such that $\rho(\mu_i) = h_i$. Then the convex combination

$$\mu = \lambda \mu_1 + (1 - \lambda)\mu_2$$

lies in $\mathcal{M}_L$ and has rotation vector $\rho(\mu) = \lambda h_1 + (1 - \lambda)h_2$. Since both μ_1 and μ_2 are minimal, we conclude that

$$\alpha(\lambda h_1 + (1 - \lambda)h_2) = \min\{A(\nu) \,|\, \nu \in \mathcal{M}_L, \; \rho(\nu) = \rho(\mu)\} \leq A(\mu) =$$
$$\int L \, d(\lambda \mu_1 + (1 - \lambda)\mu_2) = \lambda \int L \, d\mu_1 + (1 - \lambda) \int L \, d\mu_2 = \lambda \alpha(h_1) + (1 - \lambda)\alpha(h_2)$$

which proves the convexity of α. □

Since α is convex, it posseses a convex conjugate

$$\begin{aligned} \alpha^* : H^1(\mathbb{T}^n, \mathbb{R}) &\to \mathbb{R} \\ c &\mapsto \sup_{h \in H_1} (\langle c | h \rangle - \alpha(h)) \end{aligned}$$

4.2 Mañé critical value

Definition 4.2.1. *A curve $\gamma : [a, b] \to \mathbb{T}^n$ is called absolutely continuous if for every $\varepsilon > 0$ there exists $\delta > 0$ such that for every finite set of open disjoint intervals $(s_i, t_i) \subset [a, b]$ of total length less than δ, one has $\sum_i d(\gamma(t_i), \gamma(s_i)) < \varepsilon$ where d is a Riemannian metric on $\mathbb{T}^n$.*

Definition 4.2.2. *Let $L : T\mathbb{T}^n \to \mathbb{R}$ be a convex Lagrangian. The action of an absolutely continuous curve $\gamma : [a, b] \to \mathbb{T}^n$ is*

$$A_L(\gamma) := \int_a^b L(\gamma(t), \dot{\gamma}(t))\, dt$$

Given two points $x_1, x_2 \in \mathbb{T}^n$ and $T > 0$, we denote with $C_T(x_1, x_2)$ the set of absolutely continuous curve $\gamma : [0, T] \to \mathbb{R}$ with $\gamma(0) = x_1$ and $\gamma(T) = x_2$.

Definition 4.2.3. *For every $k \in \mathbb{R}$ we define*

$$\Phi_k(x_1, x_2; T) := \inf\{A_{L+k}(\gamma) \,|\, \gamma \in C_T(x_1, x_2)\}$$

The action potential Φ_k is

$$\begin{aligned} \Phi_k : \mathbb{T}^n \times \mathbb{T}^n &\to \mathbb{R} \cup \{-\infty\} \\ (x_1, x_2) &\mapsto \inf_{T>0} \Phi_k(x_1, x_2; T) \end{aligned}$$

and the critical value of L is given by

$$c(L) := \inf\{k \in \mathbb{R} \,|\, \Phi_k(x, x) > -\infty \text{ per qualche } x \in \mathbb{T}^n\}$$

The following proposition show the relation between Mañé critical value and minimal action of all the measures of $\mathcal{M}_L$, regardless of their rotation vector.

Proposition 4.2.4.

$$c(L) = -\min\{A_L(\mu) \,|\, \mu \in \mathcal{M}_L\}$$

Proof. First of all, one can show that

$$\min\{A_L(\mu) \,|\, \mu \in \mathcal{M}_L\} = \min\{A_L(\mu_\gamma) \,|\, \gamma \text{ abs. cont. curve}\}$$

where μ_γ is the probability measure equally distributed along some absolutely continuous curve γ. We prove that

$$-c(L) = \min\{A_L(\mu_\gamma) \,|\, \gamma \text{ abs. cont. curve}\}$$

For any curve γ, we have $A_{L+c(L)}(\mu_\gamma) \geq 0$ by definition of $c(L)$. Therefore

$$-c(L) \leq \min\{A_L(\mu_\gamma) \,|\, \gamma \text{ abs. cont. curve}\}$$

To prove the reversed inequality, we observe that, when $k < c(L)$, there exists a curve γ with $A_{L+k}(\mu_\gamma) < 0$, which implies

$$-k \geq \min\{A_L(\mu_\gamma) \,|\, \gamma \text{ abs. cont. curve}\}$$

and to get the result, we let k tend to $c(L)$. □

Reconsidering the definition of $\alpha^*(c)$ we have

$$\alpha^*(0) = -\min_h \min\{A_L(\mu) \,|\, \rho(\mu) = h\} = -\min\{A_L(\mu) \,|\, \mu \in \mathcal{M}_L\}$$

that gives an alternative way to describe the critical value $c(L)$.

Corollary 4.2.5. *For every closed 1-form ν on $\mathbb{T}^n$, we have*

$$c(L - \nu) = \alpha^*([\nu])$$

Moreover, if H is the Hamiltonian corresponding to L, we have

$$c(L) = \inf_{u \in C^\infty(\mathbb{T}^n, \mathbb{R})} \max_{x \in \mathbb{T}^n} H(x, du(x))$$

Remark 4.2.6 To make an example we can consider two Lagrangians on $\mathbb{T}^n$

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

where $V(x)$ is a continuous potential. Then

$$c(L^-) = \max_{x \in \mathbb{T}^n} V(x)$$
$$c(L^+) = \max_{x \in \mathbb{T}^n} \{-V(x)\} = -\min_{x \in \mathbb{T}^n} V(x)$$

that means $\|V\|_{C^0} = c(L^-) + c(L^+)$ or equivalently $\frac{1}{2}\|L^+ - L^-\|_{C^0} = c(L^-) + c(L^+)$. Considering the fact that $L^+ = H$ is the Legendre transform of L, we have $c(L^+) = c(H)$ or $c(H + h) = \alpha(h)$.

4.3 WKAM solutions

From the fact that an invariant torus is the graph of a closed 1-form ν, then ν must satisfy the equation $H(x, \nu_x) = k$ where k is a constant. Finding a smooth exact invariant torus $\operatorname{gr} du$, where $u : \mathbb{T}^n \to \mathbb{R}$ is a smooth function, is equivalent to finding a smooth solution of the time independent Hamilton-Jacobi equation

$$H(x, du(x)) = k$$

Given a continuous function $u : \mathbb{T}^n \to \mathbb{R}$, we will write

$$u \prec L + c$$

if $u(x) - u(y) \leq \Phi_c(y, x)$ for all $x, y \in \mathbb{T}^n$, where Φ_c is the action potential for the critical value

$$c = c(L)$$

Remark 4.3.1 Fathi in [Fat05] has shown that a function u satisfies $u \prec L + c$ if and only if it is Lipschitz and satisfies

$$H(x, du(x)) \leq c \quad \text{per q.o. } x \in \mathbb{T}^n$$

i.e. is a subsolution of Hamilton-Jacobi equation.

4.4 Uniqueness of WKAM solutions

Viscosity solutions and stable/unstable manifold

Here we will look to the following problem on $\mathbb{T}^d$

$$H(x, \nabla S(x)) = c \tag{4.4.1}$$

and we will try to find out the relation between the viscosity solution $S(x)$ and the stable/unstable manifold. First of all it is important to stress out the fact that this problem has been already solved by [AIPSM05]. Here we want to explain and clarify their work.
Equation (4.4.1) can be solved using viscosity methods: it is possible to solve

$$H(x, \nabla S_\varepsilon(x)) + \varepsilon \Delta S_\varepsilon(x) = c(\varepsilon) \tag{4.4.2}$$

obtaining an unique sequence of equilipschitz solutions $(S_\varepsilon)_{\varepsilon>0}$ (for an unique value $c(\varepsilon)$) that admits a convergent subsequence $(S_{\varepsilon_k})_{k\in\mathbb{N}} \to S$ where S is a solution of (4.4.1). At this point it is important to stress out the fact that exists an unique value $c \in \mathbb{R}$ such that equation (4.4.1) admits a solution, but in general this solution is not unique (obviously different solutions can differ by a constant but can also be completely different).

In the following we will make the following hypothesis on the Hamiltonian:

(i) $H : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$, $H(x,p) = \frac{p^2}{2} + V(x)$ (we will consider only mechanical Hamiltonians);

(ii) $V(x)$ has only non degenerate maxima $(x_i)_{1\le i\le m}$;

(iii) there exists only one $x_I \in \{x_i | 1 \le i \le m\}$ that minimizes $\sum_{j=1}^m \sqrt{k_j(x_i)}$ where $-k_j(x_i)$ is the j-th eigenvalue of the Hessian of V at the point x_i.

Aubry set and static classes

Definition 4.4.1. *A continuous function $S : \mathbb{T}^d \to \mathbb{R}$ is called a viscosity solution of equation (4.4.1) if it satisfies:*

(i) If v is a C^1 function and $S - v$ has a local maximum at x then

$$H(x, Dv(x)) \ge c$$

(ii) If v is a C^1 function and $S - v$ has a local minimum at x then

$$H(x, Dv(x)) \le c$$

The constant $c \in \mathbb{R}$ in equation (4.4.1) can be characterized using α Mather's function:

$$c = \alpha(0) = -\inf_{\mu}\{\int_{\mathbb{T}^d\times\mathbb{R}^d} L(x,v)d\mu(x,v)\}$$

where μ are probability measures on $\mathbb{T}^d \times \mathbb{R}^d$ invariant under the Euler-Lagrange flow of L. The action of a piecewise C^1 curve $\gamma : [0,T] \in \mathbb{T}^d$ is defined by

$$A(\gamma) = \int_0^T L(\gamma(s), \dot\gamma(s))ds$$

Definition 4.4.2. *Given $k \in \mathbb{R}$, the Peierls barrier is a function $h : \mathbb{T}^d \times \mathbb{T}^d \to \mathbb{R} \cup \{-\infty, +\infty\}$ defined by*

$$h^k(x_0, x_1) = \liminf_{T\to\infty} h^k_T(x_1, x_2)$$

where

$$h^k_T(x_0, x_1) = \inf_{\gamma}\{A(\gamma) + kT | \gamma(0) = x_0 \textit{ and } \gamma(T) = x_1\}$$

Since T is not bounded, there exists only one value of k such that h^k will be finite: that value is c the Mañé critical value.

Definition 4.4.3. *Define*

$$h_T(x_0, x_1) = h^c_T(x_0, x_1); \;\; h(x_0, x_1) = h^c(x_0, x_1)$$

and

$$\mathcal{A} = \{x \in \mathbb{T}^d | h(x,x) = 0\}$$

is the Aubry set.

Remark 4.4.4 The set $\mathcal{A}$ can be lifted in an unique way to a set $\tilde{\mathcal{A}} \subset \mathbb{T}^d \times \mathbb{R}^d$ that is invariant by Euler-Lagrange flow.

The static classes on $\mathcal{A}$ are defined by equivalence: $x \sim y$ if and only if

$$h(x,y) + h(y,x) = 0$$

Viscosity solutions are completely determined by the values taken at each static class: denote with U_i the i-th static class and choose a point x_i for each static class. Moreover assign a value $\phi_i \in \mathbb{R}$ for every i. If there exists a viscosity solution of (4.4.1) such that $S(x_i) = \phi_i$ for all i, we have $\phi_j - \phi_i \leq h(x_i, x_j)$. Viceversa if $\phi_j - \phi_i \leq h(x_i, x_j)$ for every $i, j \in [1, m]$, then there exists an unique viscosity solution $S(x)$ given by

$$S(x) = \max_i \phi_i - h(x, x_i)$$

Remark 4.4.5 Let $H(x,p) = \frac{p^2}{2} + V(x)$, where V has a finite number of maxima $(x_i)_{1 \leq i \leq m}$ which are all non degenerate. The static classes are the points x_i and $c = \max V$. We will assume that there is only one x_I such that

$$\sum_j \sqrt{k_j(x_i)} > \sum_j \sqrt{k_j(x_I)}$$

for every $i \neq I$ and $-k_j(x_i), j = 1, \dots, d$ are the eigenvalues of the Hessian of V at x_i.

Proposition 4.4.6. *If S is a viscosity solution of the Hamilton-Jacobi equation*

$$\frac{1}{2}|\nabla S(x)|^2 + V(x) = c$$

that has a local maximum at x_i, then S is C^3 in a neighbourhood of x_i and the eigenvalues of $D^2 S(x_i)$ are $-\sqrt{k_j(x_i)}$, $j = 1, \dots, d$.

Proof. S has a maximum in x_i so, using $v = S(x_i)$ in the definition of viscosity solution, we get

$$V(x_i) = \frac{1}{2}|Dv|^2 + V(x_i) \geq c = \max V(x)$$

thus x_i is a maximum of V. There exists a neighbourhood U of x_i such that for every $x \in U$, the point $(x, \nabla S(x))$ is in the stable manifold W^s of $(x_i, 0)$. Moreover $S_{|U}$ is in the same class of differentiability as V and coincides with $-h(., x_i)$. Differentiating we get

$$D^2S(x_i)D^2S(x_i) = -D^2V(x_i)$$

So if R is a matrix that diagonalizes $D^2V(x_i)$ then it also diagonalizes $D^2S(x)D^2S(x)$ and so the eigenvalues of $D^2S(x_i)$ are $-\sqrt{k_j(x_i)}$. ☐

Stochastic Lax Formula and estimates

We introduce the probability space $(\Omega, \mathcal{B}, \mathbb{P})$ with a Brownian motion $W(t)$ on the flat torus $\mathbb{T}^d$. The solution of (4.4.2) satisfies

$$S_\varepsilon(x) = \sup_v \mathbb{E}\Big(S_\varepsilon(X_\varepsilon(\tau)) - \int_0^\tau L(X_\varepsilon(s), v(s))ds - c(\varepsilon)\tau\Big) \tag{4.4.3}$$

where v is an admissible progrssively measurable control process and X_ε is the solution to the stochastic equation

$$\begin{cases} dX_\varepsilon(t) = v(t)dt + \sqrt{2\varepsilon}\,dW(t) \\ X_\varepsilon(0) = x \end{cases} \tag{4.4.4}$$

Now we show that the solutions of (4.4.2) are Lipschitz and semiconvex.

Lemma 4.4.7. *The solutions S_ε of (4.4.2) are Lipschitz and semiconvex uniformly in ε. Therefore there are always subsequences converging in the C^0 norm.*

Proof. $|c(\varepsilon)|$ is bounded independentely of ε: applying the definition of viscosity solution to $v = 0$ and x we get

$$\inf H(x, 0) \leq c(\varepsilon) \leq \sup H(x, 0)$$

By hypothesis $|\partial_x H(x, p)| \leq K(|p| + 1)$ for a constant $K > 0$. Since H is superlinear there exists $R > 0$ such that for $|p| \geq R$

$$H(x, p) \geq r + \sqrt{dK}(|p| + 1)$$

where d is the dimension of the torus. Let $w = |DS_\varepsilon|^2$ then

$$Dw = 2D^2S_\varepsilon DS_\varepsilon \tag{4.4.5}$$

$$\Delta w = 2\text{Tr}(D^2S_\varepsilon)^2 + 2D(\Delta S_\varepsilon) \cdot DS_\varepsilon \tag{4.4.6}$$

Then we get

$$\partial_x H \cdot DS_\varepsilon + \frac{1}{2}\partial_p H \cdot Dw + \frac{\varepsilon}{2}\Delta w - \varepsilon \text{Tr}(D^2S_\varepsilon)^2 = 0$$

Let $x_0 \in \mathbb{T}^d$ be a point where w attains its maximum, then $Dw(x_0) = 0$ and $\Delta w(x_0) \leq 0$. We have

$$(H(x_0, DS_\varepsilon) - c(\varepsilon))^2 \leq \varepsilon d K(|DS_\varepsilon| + 1)|DS_\varepsilon|$$

□

Some useful propositions

Fathi and Siconolfi showed the existence of a C^1 critical subsolution of HJ equation, i.e.

$$H(x, \nabla f) \leq c$$

Moreover, they found that such an f can be constructed so that $H(x, \nabla f) < c$ outside $\mathcal{A}$ (the Aubry set). As a consequence (Legendre inequality):

$$L(x, v) + c - \nabla f(x) \cdot v \geq L(x, v) + H(x, \nabla f) - \nabla f(x) \cdot v \geq 0 \tag{4.4.7}$$

for all $(x, v) \in \mathbb{T}^d \times \mathbb{R}^d$ and it is equal to 0 if $(x, v) \in \mathcal{A}$. In the following we will assume that the static classes consist only of a finite number of periodic hyperbolic orbit $\gamma_i : [0, T_i] \to \mathbb{T}^d$ for $1 \leq i \leq m$.

Lemma 4.4.8. *Let S be a viscosity solution of (4.4.1) and define $\varphi = S - f$ and also*

$$\tilde{h}(x, y) = h(x, y) + f(x) - f(y)$$

Then

(i) $\tilde{h}(x, y) \leq \tilde{h}(x, z) + \tilde{h}(z, y)$*;*

(ii) $\tilde{h}(x, y) \geq 0$ *and* $\tilde{h}(x, y) = 0$ *if and only if* $x, y \in \gamma_i$ *for some* i*;*

(iii) φ *is constant on* γ_i *for every* i*;*

(iv) if $x \in \mathbb{T}^d$ *is a local maximum of* φ *then exists* i *such that* $x \in \gamma_i$*.*

Proof. (i) $\tilde{h}(x, y) = h(x, y) + f(x) - f(y) \leq h(x, z) + h(z, y) + f(z) - f(z) + f(x) - f(y) = \tilde{h}(x, z) + \tilde{h}(z, y)$.

(ii)

$$\begin{aligned}\tilde{h}(x, y) = h(x, y) + f(x) - f(y) &= \lim_{T \to \infty} \inf_{\gamma} \int_0^T \Big[L(\gamma(s), \dot{\gamma}(s)) + c\Big] ds + f(x) - f(y) \\ &= \lim_{T \to \infty} \inf_{\gamma} \int_0^T L(\gamma(s), \dot{\gamma}(s)) + c + \nabla f(\gamma(s)) \cdot \dot{\gamma}(s) ds\end{aligned}$$

and we have $\tilde{h}(x, y) \geq 0$ from (4.4.7). If x and y are in the same γ_i then $L + c + \nabla f \cdot \dot{\gamma} = 0$ and we have $\tilde{h}(x, y) = 0$.

(iii) We use

$$S(\gamma_i(T)) - S(\gamma_i(0)) = \int_0^T L(\gamma_i(t), \dot{\gamma}_i(t))dt + cT$$

From this we get

$$g(\gamma_i(T)) - g(\gamma_i(0)) = \int_0^T (L(\gamma_i(t), \dot{\gamma}_i(t))) + c - \nabla f(\gamma_i(t), \dot{\gamma}_i(t))dt$$

Since $L + c - \nabla f$ is zero on the Aubry set (that contains every γ_i), we have that g is constant along γ_i.

(iv) S is a viscosity solution of (4.4.1) so, if x is a local maximum of g, then

$$H(x, Df(x)) \geq c$$

but this is true only if $x \in \mathcal{A}$.

□

Proposition 4.4.9. *If S is a viscosity solution to the Hamilton-Jacobi equation (4.4.1) and $g = S - f$ has a local maximum at γ_i, then there is a neighbourhood U of γ_i such that*

$$S(x) = S(x_i) - h(x, x_i)$$

for $x \in U$. This implies that $(x, \nabla S(x))$ belongs to the stable manifold $(x_i, 0)$ under the Hamiltonian flow, and that S is C^3 on U.

Proof. Let U be a neighbourhood of x_i on which x_i is a local maximum of g. Then for every j we have

$$g(x_i) = g(x_i) - \tilde{h}(x_i, x_i) \geq g(x_j) - \tilde{h}(x_i, x_j) \tag{4.4.8}$$

Remember that g and $\tilde{h}$ are continuous so, if the inequality is strict for all $j \neq i$, there exists a neighbourhood of γ_i where

$$g(x) = \max_k \{g(x_k) - \tilde{h}(x, x_k)\} = g(x_i) - \tilde{h}(x, x_i)$$

and, using the definition of g and $\tilde{h}$, we get $S(x) = S(x_i) - h(x, x_i)$.
It is more difficult to show this when the equality in (4.4.8) occurs for some $j \neq i$. We start choosing $y \in \partial U$ such that $h(x_i, y) + h(y, x_j) = h(x_i, x_j)$. Let $\gamma_T : [0, T] \to \mathbb{T}^d$ be a curve joining x_i and x_j and achieving

$$h_T(x_i, x_j) = \inf\{A(\gamma) + cT | \gamma : [0, T] \to \mathbb{T}^d \text{ joins } x_i \text{ and } x_j\}$$

Let us define T_U the smallest time such that $\gamma_T(T_U) \notin U$ and $y_T = \gamma_T(T_U) \in \partial U$ the first point of intersection. Now we show that both T_U and $T - T_U$ tends to infinity when $T \to \infty$: this follows from the fact that $\dot{\gamma_T}(0) \to \dot{\gamma_i}(0)$ and $\dot{\gamma_T}(T) \to \dot{\gamma_j}(0)$. In fact let v a limit point of $\dot{\gamma_T}(0)$ and let $(\gamma(t), \dot{\gamma}(t))_{t\geq 0}$ be the Euler-Lagrange flow of (x_i, v). Using that

$$h_T(x_i, x_j) - h_{T-1}(\gamma_T(1), x_j) = A(\gamma_{T|[0,1]})$$

and letting $T \to \infty$, we get

$$h(x_i, x_j) - h(\gamma(1), x_j) = A(\gamma_{|[0,1]})$$

Moreover

$$h(\gamma_i(-1), x_j) - h(x_i, x_j) = A(\gamma_{i|[-1,0]})$$

so

$$h(\gamma_i(-1), x_j) - h(\gamma(1), x_j) = A(\gamma_{|[0,1]}) + A(\gamma_{i|[-1,0]})$$

□

Lemma 4.4.10. *If S is a viscosity solution of (4.4.1) such that $g = S - f$ has only one maximum at the orbit γ_I, then*

$$S(x) = S(x_I) - h(x, x_I)$$

Proof. We assume that $I = 1$, $g(x_1) = 0 = -\tilde{h}(x_1, x_1)$ and $g(x_1) \geq g(x_2) \geq \ldots \geq g(x_m)$. We use induction: we assume that $g(x_l) = -\tilde{h}(x_l, x_1)$ for $l \leq i$, and we prove □

Next we introduce the following

$$\lambda_i := \frac{1}{T_i}\int_0^{T_i} \Delta h_i(\gamma_i(t))dt = \frac{1}{T_i}\int_0^{T_i} \Delta h(\gamma_i(t), x_i)dt$$

(where $x_i = \gamma_i(0)$), for $i \in \{1, \ldots, m\}$. We assume there is only one i for which λ_i is minimal: we call it I.

Lemma 4.4.11.

$$c'_+(0) := \liminf_{\varepsilon\to 0^+} \frac{c(\varepsilon) - c(0)}{\varepsilon} \geq -\lambda_I$$

Proof. □

Lemma 4.4.12. *Suppose that $g = S - f$ has a local maximum at γ_i. Then $i = I$ and*

$$\lim_{n\to\infty} \frac{c(\varepsilon_n) - c(0)}{\varepsilon_n} = -\lambda_I$$

Proof. □

The fundamental theorem

We recall here the hypothesis that we need:

(i) there exists only one static class γ_I such that

$$\lambda_I = \min_{1 \leq i \leq m} \lambda_i$$

(ii) $\frac{\partial_x H}{|p|+1}$ is uniformly bounded.

Under these conditions we state and prove the following:

Theorem 4.4.13. *The solution S_ε of (4.4.2), normalized imposing $S_\varepsilon(x_I) = 0$, converges uniformly to $-h_I(x) = -h_I(x, x_I)$ as $\varepsilon \to 0$.*

Proof. Let f be a C^1 critical subsolution that we suppose strict outside the static classes and let S_{ε_n} be a sequence of solutions of (4.4.2). Using Lemma 4.4.7 we know that there exists a convergent subsequence $S_{\varepsilon_{n_k}}$; we call S_0 its limit. By Lemma 4.4.12 we have that the unique place where $S_0 - f$ can have a local maximum is at γ_I. So we have

$$S_0(x) = S_0(x_I) - h(x, x_I)$$

(from Lemma 4.4.10). But $S_{\varepsilon_{n_k}}(x_I) = 0$ (from the normalization condition) that implies $S_0(x_I) = 0$ and so

$$S_0(x) = -h(x, x_I)$$

□

We showed that the unique solution $S_0(x)$ coincides with $-h(x, x_I)$ that is the "weak" generating function of the stable manifold (see Proposition 4.4.6), and this holds true for every convergent subsequence $S_{\varepsilon_{n_k}}$.

4.5 Quantum Unique Ergodicity (QUE)

Let $a \in C_c^\infty(TM)$. Egorov's theorem states that for t fixed, one has

$$\left\| \exp\left(-\frac{it\varepsilon}{2}\Delta\right) \mathrm{Op}_\varepsilon(a) \exp\left(\frac{it\varepsilon}{2}\Delta\right) - \mathrm{Op}_\varepsilon(a \circ g^t) \right\|_{L^2(M)} = O(\varepsilon)$$

for $\varepsilon \to 0$, where g^t is the geodetic flow (we assume that it is "chaotic" in some sense: hyperbolic, ergodic, mixing...) on a Riemannian manifold M (we can think of $M = \mathbb{T}^n$). We consider the problem

$$-\varepsilon^2 \Delta \psi_\varepsilon = \psi_\varepsilon \tag{4.5.1}$$

when $\varepsilon \to 0$ (high energies) and an orthonormal basis of $L^2(M) = L^2(M, dVol)$ where Vol is the volume measure of M. Then every wave function

$$|\psi_\varepsilon(x)|^2 dVol(x)$$

defines a probability measure on M that can be lifted to TM considering the distributions

$$\nu_\varepsilon(a) = \langle \mathrm{Op}_\varepsilon(a)\psi_\varepsilon, \psi_\varepsilon \rangle_{L^2(M)}$$

called Husimi distributions (choosing the right quantization these are effectively probability measures). The limit ν_0 of a convergent subsequence is again a probability measure on $S^1M \subset TM$ (S^1M is the unitary sphere of TM). By Egorov's theorem ν_0 is flow-invariant. We will call these measures *semiclassical measures*. The problem is to understand which measures are semiclassical measures (more precisely: which measures are the limit of a subsequence of Husimi's measures?). The following theorem gives an answer to this question.

Theorem 4.5.1 (Snirelman, Zelditch, Colin de Verdière)**.** *Let g^t ergodic for the Lioville normalized measure L on S^1M. Then there exists $J \subset \mathbb{N}$ of density 1 such that*

$$\nu_j \to L$$

for $j \in J$.

Snirelman's theorem tells us that "almost all" subsequences converge to Liouville's measure. QUE conjecture (Quantum Unique Ergodicity) states: if M has negative sectional curvature then all subsequences converge to L.
We return now to the problem of determine a couple $(a(t,x), S(t,x))$ of solutions of

$$\begin{cases} \partial_t S + H(x, \nabla S) = \frac{\varepsilon^2}{2}\frac{\Delta A}{A} \\ S(0,x) = S_0(x) \\ \partial_t P + \mathrm{div}(P\nabla S) = 0, \quad \sqrt{P} = A \\ P(0,x) = P_0(x) \end{cases} \tag{4.5.2}$$

and suppose that

$$\lim_{t\to\infty} -\frac{S_\varepsilon(t,x)}{t} = c_\varepsilon[0] \overset{\varepsilon\to 0}{\to} c_0[0] = \max V \tag{4.5.3}$$

holds true. As we have already seen

$$c_\varepsilon[0] = -\inf_{\mu_\varepsilon}\Big\{\int L\mu_\varepsilon\Big\}$$

and suppose that the infimum is effectively reached, i.e. there exists a measure μ_ε such that

$$\int L\mu_\varepsilon = c_\varepsilon[0] \overset{\varepsilon\to 0}{\to} c_0[0] = \max V = \int L\mu$$

This means: semiclassical measures seem to be Mather's measures, the ones that minimize the action.
Let $\psi \in L^2(\mathbb{T}^n)$ and suppose to compute the mean value $\langle\psi|A\psi\rangle$ for some observable A. Quantum

observables are represented by pseudo-differrential operators with principal simbol of class C^∞. Weyl quantization procedure will give

$$\langle\psi|A\psi\rangle = \sum_{p\in\varepsilon\mathbb{Z}^n}\int_{\mathbb{T}^n}\int_{\mathbb{T}^n} a(x,2\pi p)\bar{\psi}\left(x+\frac{y}{2}\right)\psi\left(x-\frac{y}{2}\right)e^{-2\pi ipy/\varepsilon}dydx$$

Wigner measures on $T^*\mathbb{T}^n$ are defined by the density

$$W_\varepsilon(x,p) = \int_{\mathbb{T}^n}\bar{\psi}(x+\frac{y}{2})\psi(x-\frac{y}{2})e^{-2\pi ipy/\varepsilon}dy$$

for all $p\in\varepsilon\mathbb{Z}^n$. In this way

$$\langle\psi|A\psi\rangle = \sum_{p\in\varepsilon\mathbb{Z}^n}\int_{\mathbb{T}^n} a(x,2\pi p)W_\varepsilon(x,p)$$

Wigner measures have the following properties.

Proposition 4.5.2. *(i) Let ψ smooth and such that*

$$\int_{\mathbb{T}^n}|\psi|^2 = 1$$

Then

$$\sum_{p\in\varepsilon\mathbb{Z}^n}\int_{\mathbb{T}^n} W_\varepsilon(x,p) = 1$$

(ii) Let ψ a solution of Schrödinger equation

$$H\psi = E\psi$$

then

$$\sum_{p\in\varepsilon\mathbb{Z}^n}\int_{\mathbb{T}^n}\Big(\frac{|2\pi p|^2}{2}+V(x)\Big)W_\varepsilon(x,p) = E$$

(iii) Let $(\psi_\varepsilon)_\varepsilon$ a sequence of solutions of

$$H\psi_\varepsilon = E_\varepsilon\psi_\varepsilon$$

with E_ε bounded. Then, eventually considering a subsequence, W_ε converges weakly to a measure W_0 for $\varepsilon\to 0$.

(iv) W_0 is invariant for the dynamic, i.e.

$$\{W_0,H\} = p\cdot\nabla_x W_0 - \nabla_x V\cdot\nabla_p W_0 = 0$$

It is clear that the action

$$\int_{\mathbb{T}^n} \frac{\varepsilon^2}{2}|\nabla\psi|^2 - V(x)|\psi|^2$$

can be rewritten as

$$\sum_{p\in\varepsilon\mathbb{Z}^n} \int_{\mathbb{T}^n}\int_{\mathbb{T}^n} \left[\frac{|2\pi p|^2}{2} - V(x)\right] \bar{\psi}\left(x+\frac{y}{2}\right)\psi\left(x-\frac{y}{2}\right) e^{-2\pi i p y/\varepsilon} dy dx$$

In general Wigner measures are not positive: to make them positive we must consider the measures

$$\widetilde{W}_\varepsilon = \zeta_\varepsilon * W_\varepsilon$$

where

$$\zeta_\varepsilon(x,p) = C\varepsilon^n e^{-2\pi(|x|^2+|p|^2)/\varepsilon}$$

and the constant C is such that

$$\sum_{p\in\varepsilon\mathbb{Z}^n} \int_{\mathbb{T}^n} \zeta_\varepsilon(x,p)dx = 1$$

The $\widetilde{W}_\varepsilon$ are called Husimi measures. Moreover the $\widetilde{W}_\varepsilon$ converge to a positive probability measure.

Theorem 4.5.3. *(i) Let $\widetilde{W}_\varepsilon$ a Husimi measure that minimizes the action. Then for $\varepsilon \to 0$*

$$\int_{T^*\mathbb{T}^n} \frac{|p|^2}{2} - V(x)d\widetilde{W}_\varepsilon \to \int_{T^*\mathbb{T}^n} \frac{|p|^2}{2} - V(x)d\widetilde{W}_0$$

(ii) $\widetilde{W}_0$ is a Mather measure.

Appendix A

Stationary phase method

Since we will encounter the semiclassical Fourier Transform and it will be an integral of the type

$$\int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}\langle x,\xi\rangle} u(x)\, dx$$

it will be very important to understand what happen in the limit $\varepsilon \to 0$.

A.1 Stationary phase method in dimension one

Our pourpose is to study the asymptotic behaviour of

$$I(\varepsilon) = \int_{\mathbb{R}} u(x) e^{\frac{\mathrm{i}}{\varepsilon} f(x)}\, dx$$

when $\varepsilon \to 0$ (in the semiclassical regime) and u and f are sufficently smooth. We want to show that the integral is "concentrated" around the points where f is stationary. More precisely, it is possible to show that:

(i) if f has not any critical point in the support of u, then $I(\varepsilon) \sim O(\varepsilon^{\infty})$;

(ii) if f has only one non degenerate critical point x_0 in the support of u, then

$$I(\varepsilon) \sim (2\pi\varepsilon)^{1/2} \frac{e^{\mathrm{i}\sigma\frac{\pi}{4}}}{|f''(x_0)|^{\frac{1}{2}}} e^{\frac{\mathrm{i}}{\varepsilon} f(x_0)} u(x_0)$$

where $\sigma = \operatorname{sgn} f''(x_0)$ is the sign of the second derivative of f in x_0.

We start giving the following definition.

Definition A.1.1. *Let $u \in C_c^{\infty}(\mathbb{R}), f \in C^{\infty}(\mathbb{R})$, we define for $\varepsilon > 0$*

$$I(\varepsilon) = \int_{\mathbb{R}} e^{\frac{\mathrm{i}}{\varepsilon} f(x)} u(x)\, dx \tag{A.1.1}$$

Remark A.1.2 Before stating the main results, we want to clarify the notations. When we write $I(\varepsilon) \sim O(\varepsilon^\infty)$ (or equivalently $I(\varepsilon) = O(\varepsilon^\infty)$), we mean that for every $N \in \mathbb{N}$, there exists a constant K_N such that

$$|I(\varepsilon)| \leq K_N \varepsilon^N$$

for all $0 < \varepsilon \leq \varepsilon_0$ for a fixed $\varepsilon_0 > 0$.

Proposition A.1.3. *If $f'(x) \neq 0$ for all $x \in K = supp\,(u)$, then $I(\varepsilon) = O(\varepsilon^\infty)$ for $\varepsilon \to 0$.*

Proof. Fix $N \in \mathbb{N}$: this will be the number of times we will integrate by parts. Note that, since $f' \neq 0$, the differential operator

$$\widetilde{\partial} := \frac{\varepsilon}{\mathrm{i}} \frac{1}{f'} \partial_x$$

is well defined. It is trivial to see that $\widetilde{\partial} e^{\frac{\mathrm{i}}{\varepsilon} f} = e^{\frac{\mathrm{i}}{\varepsilon} f}$. This implies that $\widetilde{\partial}^N e^{\frac{\mathrm{i}}{\varepsilon} f} = e^{\frac{\mathrm{i}}{\varepsilon} f}$ and consequently

$$|I(\varepsilon)| = \left| \int_{\mathbb{R}} \widetilde{\partial}^N \left(e^{\frac{\mathrm{i}}{\varepsilon} f(x)} \right) u(x) \right| = \left| \int_{\mathbb{R}} e^{\frac{\mathrm{i}}{\varepsilon} f(x)} \left(\widetilde{\partial}^N \right)^* u(x) \right|$$

where $\widetilde{\partial}^*$ is the adjoint of $\widetilde{\partial}$ and it is given by

$$\widetilde{\partial}^* u = -\frac{\varepsilon}{\mathrm{i}} \partial_x \left(\frac{u}{f'} \right)$$

From the fact that u is smooth and compactly supported we have that the last expression is of size ε. Thus $|I(\varepsilon)| \leq K_N \varepsilon^N$ as required. □

The previous proposition tells us that if the phase has no stationary point in the support of the amplitude than the integral $I(\varepsilon)$ goes to 0 more rapidly than any power of ε. What happens if $f' = 0$ at one point x_0 in the support of u? The next theorem gives the answer.

Theorem A.1.4. *Take $u \in C_c^\infty(\mathbb{R})$ and suppose that exist $x_0 \in K = supp\,(u)$ such that*

$$f'(x_0) = 0, \quad f''(x_0) \neq 0 \tag{A.1.2}$$

and $f'(x) \neq 0$ for all $x \in supp\,(u) \setminus \{x_0\}$. Then there exist for every $k \in \mathbb{N}$, a differential operator $A_{2k}(x, D)$ of order less or equal than $2k$ such that for all $N \in \mathbb{N}$ one has

$$\left| I(\varepsilon) - \left(\sum_{k=1}^{N-1} A_{2k}(x, D) a(x_0) \varepsilon^{k+\frac{1}{2}} \right) e^{\frac{\mathrm{i}}{\varepsilon} f(x_0)} \right| \leq C_N \varepsilon^{N+\frac{1}{2}} \sum_{0 \leq m \leq 2N+2} \sup |a^{(m)}| \tag{A.1.3}$$

where the constant C_N depends on K.
In particular

$$A_0 = (2\pi)^{1/2} |f''(x_0)|^{-1/2} e^{\frac{\mathrm{i}\pi}{4} \operatorname{sgn} f''(x_0)} \tag{A.1.4}$$

and as a consequence

$$I(\varepsilon) = (2\pi\varepsilon)^{1/2}|f''(x_0)|^{-1/2} e^{\frac{i\pi}{4}\operatorname{sgn} f''(x_0)} e^{\frac{i}{\varepsilon}f(x_0)} a(x_0) + O(\varepsilon^{3/2}) \tag{A.1.5}$$

Proof. We assume (without loss of generality) $x_0 = 0$ and $f(0) = 0$. We can write $f(x) = \frac{1}{2}g(x)x^2$ where

$$g(x) = 2\int_0^1 (1-t) f''(tx)\, dt$$

Clearly one has $g(0) = f''(0) \neq 0$ and with this condition we can make a change of variables

$$y = |g(x)|^{1/2} x$$

near $x = 0$. Now we take a smooth function χ with $0 \leq \chi \leq 1$ and $\chi = 1$ in a neighborhood of 0 and such that $\operatorname{sgn} f''(x) = \operatorname{sgn} f''(0) \neq 0$ on $\operatorname{supp}(\chi)$. Then using Proposition (A.1.3) and the previous change of variables

$$I(\varepsilon) = \int_{\mathbb{R}} e^{\frac{i}{\varepsilon}f(x)} \chi(x) a(x)\, dx + \int_{\mathbb{R}} e^{\frac{i}{\varepsilon}f(x)} (1-\chi(x)) a(x)\, dx \tag{A.1.6}$$

$$= \int_{\mathbb{R}} e^{\frac{i\sigma}{2\varepsilon}y^2} u(y)\, dy + O(\varepsilon^\infty) \tag{A.1.7}$$

where $\sigma = \operatorname{sgn} f''(0) = \pm 1$ and $u(y) = \chi(x(y)) a(x(y)) |\partial_y x|$. Applying Fourier Transform the integral becomes

$$I(\varepsilon) = \left(\frac{\varepsilon}{2\pi}\right)^{1/2} e^{\frac{i\pi\sigma}{4}} \int_{\mathbb{R}} e^{-\frac{i\sigma\varepsilon\xi^2}{2}} \widehat{u}(\xi)\, d\xi + O(\varepsilon^\infty) \tag{A.1.8}$$

Now we define

$$J(\varepsilon, u) = \int_{\mathbb{R}} e^{-\frac{i\sigma\varepsilon\xi^2}{2}} \widehat{u}(\xi)\, d\xi$$

with the "initial" condition $J(0, u) = 2\pi u(0)$. Then observing that

$$\partial_\varepsilon J(\varepsilon, u) = \int_{\mathbb{R}} e^{-\frac{i\sigma\varepsilon\xi^2}{2}} \left(\frac{\sigma\xi^2}{2i}\widehat{u}(\xi)\right) d\xi = J(\varepsilon, \widetilde{\partial} u)$$

where $\widetilde{\partial} = \frac{\sigma}{2i}\partial^2$. By induction

$$\partial_\varepsilon^k J(\varepsilon, u) = J(\varepsilon, \widetilde{\partial}^k u)$$

so that, computing Taylor expansion, we have

$$J(\varepsilon, u) = \sum_{k=0}^{N-1} \frac{\varepsilon^k}{k!} J(0, \widetilde{\partial}^k u) + \frac{\varepsilon^N}{N!} R_N(\varepsilon, u)$$

where the remainder is given by

$$R_N(\varepsilon, u) = N\int_0^1 (1-t)^{N-1} J(t\varepsilon, \widetilde{\partial}^N u)\, dt$$

and the following estimate holds

$$|R_N| \leq C_N \|\widehat{\widetilde{\partial}^N u}\|_{L^1} \leq C_N \sum_{0\leq k\leq 2} \sup_{\mathbb{R}} |\partial^k (\widetilde{\partial}^N u)|$$

The last step is to find the expression for the terms in the expansion: from the definition of J we have

$$\varepsilon^k J(0, \widetilde{\partial}^k u) = \varepsilon^2 \widetilde{\partial}^k u(0) = \left(\frac{\varepsilon}{2\mathrm{i}}\right)^k u^{(2k)}(0)$$

and using the fact that $u = \chi(x(y))a(x(y))|\partial_y x|$, one gets the expansion in (A.1.3).

□

A.2 Stationary phase in higher dimensions

Theorem A.2.1. *Let $K \subset \mathbb{R}^d$ be a compact set, X an open neighborhood of K and $j, k \in \mathbb{Z}^+$. If $u \in C_0^k(K)$, $f \in C^{k+1}(X)$ and $\operatorname{Im} f \geq 0$ in X, then*

$$\varepsilon^{-(j+k)} \left| \int e^{\frac{\mathrm{i}}{\varepsilon} f(x)} (\operatorname{Im} f(x))^j u(x)\, dx \right| \leq C \sum_{|\alpha|\leq k} \sup |D^\alpha u| (|\nabla f|^2 + \operatorname{Im} f)^{|\alpha|/2 - k} \tag{A.2.1}$$

When $f(x)$ is real valued the previous relation reduces to

$$\varepsilon^{-k} \left| \int e^{\frac{\mathrm{i}}{\varepsilon} f(x)} u(x)\, dx \right| \leq C \sum_{|\alpha|\leq k} \sup |D^\alpha u| |\nabla f|^{|\alpha| - 2k}$$

The previous theorem asserts that the integral decreases faster than any power of ε for $\varepsilon \to 0$ if there are no points with $\nabla f(x) = 0$ and $\operatorname{Im} f = 0$ in the support of u.

Lemma A.2.2. *(i) Let*

$$I(\varepsilon) = \left(\frac{1}{2\pi\varepsilon}\right)^{k/2} \int_{\mathbb{R}^k} e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x,\theta)} a(x,\theta) d\theta$$

and assume that $\operatorname{Im}\varphi(x,\theta) \geq 0$ and

$$|a(x,\theta)| \leq \widetilde{C}_N \left(\operatorname{Im}\varphi(x,\theta)\right)^N \tag{A.2.2}$$

Then we have for $\varepsilon \leq 1$

$$\left| e^{\frac{\mathrm{i}}{\varepsilon}\varphi(x,\theta)} a(x,\theta) \right| \leq C_N \varepsilon^N \tag{A.2.3}$$

(ii) Let

$$I(\varepsilon) = \left(\frac{1}{2\pi\varepsilon}\right)^{k/2} \int_{\mathbb{R}^k} e^{\frac{\mathrm{i}}{\varepsilon}\psi(t,x,\theta)} a(t,x,\theta) d\theta$$

and assume that $\operatorname{Im}\psi(t,x,\theta) = \varphi(x,\theta) \operatorname{Im}\zeta(t) \geq 0$ and

$$|a(t,x,\theta)| \leq \widetilde{C}_N \left(\operatorname{Im}\psi(t,x,\theta)\right)^N = \widetilde{C}_N \left(\operatorname{Im}\zeta(t)\right)^N \left(\varphi(x,\theta)\right)^N \tag{A.2.4}$$

Then we have for $\varepsilon \leq 1$

$$\left| e^{\frac{i}{\varepsilon}\psi(t,x,\theta)} a(t,x,\theta) \right| \leq C_N \varepsilon^N \left(\operatorname{Im}\zeta(t)\right)^N \tag{A.2.5}$$

Proof. (i) We can make the following estimates

$$\left| e^{\frac{i}{\varepsilon}\varphi(x,\theta)} a(x,\theta) \right| \leq e^{-\frac{1}{\varepsilon}\operatorname{Im}\varphi(x,\theta)} |a(x,\theta)| \leq \widetilde{C}_N \left(\operatorname{Im}\varphi(x,\theta)\right)^N e^{-\frac{1}{\varepsilon}\operatorname{Im}\varphi(x,\theta)} \tag{A.2.6}$$

where in the last inequality we have used (A.2.2). The following simple inequality holds true for $y > 0$ and $0 < \varepsilon < 1$:

$$e^{-\frac{1}{\varepsilon}y} y^N \leq \max_{x \geq 0}\{e^{-x}x^N\} \frac{1}{\varepsilon}^{-N}$$

Applying it to (A.2.6) gives the result.

(ii) Use the same arguments as before (but multiplying where necessary by $\operatorname{Im}\zeta(t)$).

□

A.3 Gauss transform

Here we study the problem of estimating integrals of the form

$$\int e^{-\langle x, Ax\rangle/2} f(x) dx$$

where $\operatorname{Re} Q \geq 0$ and f is smooth.

Lemma A.3.1. *Let A be a $n \times n$ matrix such that $\operatorname{Re} A \geq 0$ and $f \in \mathcal{S}(\mathbb{R}^n)$ then*

$$\int e^{-\langle x, Ax\rangle/2} f(x) dx = \frac{1}{\sqrt{\det(A/2\pi)}} e^{-\langle D_x, A^{-1}D_x\rangle/2} f(x)_{|x=0} \tag{A.3.1}$$

where

$$e^{-\langle D_x, A^{-1}D_x\rangle/2} e^{i\langle x,\xi\rangle} := e^{-\langle \xi, A^{-1}\xi\rangle/2} e^{i\langle x,\xi\rangle}$$

Proof. We use the Fourier Transform of a Gaussian

$$e^{-\langle x, Ax\rangle/2} = \frac{1}{(2\pi)^n} \frac{1}{\sqrt{\det(A/2\pi)}} \int e^{-\langle \xi, A^{-1}\xi\rangle/2} e^{i\langle x,\xi\rangle} d\xi$$

and the Fourier inversion formula

$$\begin{aligned}
\int e^{-\langle x,Ax\rangle/2} f(x)dx &= \frac{1}{(2\pi)^n}\frac{1}{\sqrt{\det(A/2\pi)}}\int\int e^{-\langle \xi,A^{-1}\xi\rangle/2}e^{\mathrm{i}\langle x,\xi\rangle}f(x)dxd\xi \\
&= \frac{1}{\sqrt{\det(A/2\pi)}}\int e^{-\langle \xi,A^{-1}\xi\rangle/2}\check{f}(\xi)d\xi \\
&= \frac{1}{\sqrt{\det(A/2\pi)}}\int e^{-\langle D_x,A^{-1}D_x\rangle/2}e^{-\mathrm{i}\langle x,\xi\rangle}\check{f}(\xi)d\xi_{|x=0} \\
&= \frac{1}{\sqrt{\det(A/2\pi)}}e^{-\langle D_x,A^{-1}D_x\rangle/2}\int e^{-\mathrm{i}\langle x,\xi\rangle}\check{f}(\xi)d\xi_{|x=0} \\
&= \frac{1}{\sqrt{\det(A/2\pi)}}[e^{-\langle D_x,A^{-1}D_x\rangle/2}f](0)
\end{aligned}$$

□

A.4 PseudoDifferential Operators (PDO)

Ler $\mathcal{A}:\mathcal{S}'(\mathbb{R}^d)\to\mathcal{S}'(\mathbb{R}^d)$ an operator, we want to see its action on a plane wave $e_\xi(x)=e^{i\langle x,\xi\rangle}$ where $\xi\in\mathbb{R}^d$ is the momentum. We will get

$$\mathcal{A}e_\xi(x)=a(x,\xi)e_\xi(x)$$

where $a(x,\xi)\in S'(\mathbb{R}^d\times\mathbb{R}^d)$ is a distribution on the phase space. For a generic function u, we expand it in plane waves and using the inverse Fourier Transform, we get

$$\mathcal{A}u(x)=\frac{1}{(2\pi)^d}\int e^{i\langle x,\xi\rangle}a(x,\xi)\widehat{u}(\xi)\,d\xi$$

The distribution $a(x,\xi)$ is usually called the (right) symbol of the operator $\mathcal{A}$. We note here that the semiclassical limit correspond (in this case) to the limit $\|\xi\|\to\infty$. In order for this limit to exists, we have to impose some conditions on the symbol $a(x,\xi)$.

Definition A.4.1. *We will say that the function $a\in C^\infty(\mathbb{R}^d\times\mathbb{R}^d)$ is a symbol of order m if there exists a constant $C_{\alpha\beta}>0$ such that*

$$\left|D_x^\alpha D_\xi^\beta a(x,\xi)\right|\le C_{\alpha\beta}(1+|\xi|)^{m-|\beta|} \tag{A.4.1}$$

for all $\alpha,\beta\in\mathbb{Z}^d$. The space of symbols of order m is denoted by

$$S^m(\mathbb{R}^d\times\mathbb{R}^d)=\{a\in C^\infty(\mathbb{R}^d\times\mathbb{R}^d)\,|\,a\text{ is a symbol of order }m\}$$

We observe here that the smallest constant $C_{\alpha\beta}$ in (A.4.1) define a family of seminorms on the space of symbols, making it a Fréchet space. We have to extend the previous definition to the semiclassical symbols.

Definition A.4.2. *We define the set of semiclassical symbols of order m and degree l as*

$$\Sigma^{m,l} = \{a_\varepsilon(x,\xi) = \varepsilon^l \sum_{j=0}^{\infty} \varepsilon^j a_j(x,\xi),\ a_j \in \Sigma^{m-j}\}$$

The previous definition means that a_ε is a semiclassical symbol if

$$a_\varepsilon(x,\xi) - \varepsilon^l \sum_{j=0}^{M-1} \varepsilon^j a_j(x,\xi) \in \varepsilon^{l+M}\Sigma^{m-M}$$

for all M and uniformly in ε.

Appendix B

Quantization

B.1 Introduction

On the notations: we will follow [EZ03] and we will work mainly on $\mathbb{R}^{2n}$ with coordinates (x, ξ). We will consider $\mathbb{R}^{2n}$ as a symplectic manifold with the bilinear antisymmetric form ω given by

$$\omega(u, v) = \langle \xi, y \rangle - \langle x, \eta \rangle \tag{B.1.1}$$

where $u = (x, \xi)$ and $v = (y, \eta)$ are two elements of $\mathbb{R}^{2n}$. Useful notations will be

$$\langle x \rangle = (1 + |x|)^{\frac{1}{2}} \tag{B.1.2}$$

and

$$D^\alpha = \frac{1}{\mathrm{i}^{|\alpha|}} \partial^\alpha \tag{B.1.3}$$

We will use functions in the Schwartz space.

Definition B.1.1. *The Schwartz space is defined as*

$$\mathcal{S}(\mathbb{R}^n) = \{u \in C^\infty(\mathbb{R}^n) | \sup_{\mathbb{R}^n} |x^\alpha \partial^\beta u| < \infty \text{ for all multi-indices } \alpha, \beta\} \tag{B.1.4}$$

and for every pair of α, β, we define the following seminorm

$$|u|_{\alpha,\beta} = \sup_{\mathbb{R}^n} |x^\alpha \partial^\beta u| \tag{B.1.5}$$

In particular we will say that $u_j \to u$ in $\mathcal{S}(\mathbb{R}^n)$ if

$$|u_j - u|_{\alpha,\beta} \to 0$$

for all α, β.

Definition B.1.2. *If $u \in \mathcal{S}(\mathbb{R}^n)$ we define its Fourier transform as*

$$\mathcal{F}u(\xi) = \widehat{u}(\xi) = \int_{\mathbb{R}^n} e^{-\mathrm{i}\langle x,\xi\rangle} u(x)\, dx \tag{B.1.6}$$

We define also the semiclassical Fourier transform for $\varepsilon > 0$

$$\mathcal{F}_\varepsilon u(\xi) = \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x,\xi\rangle} u(x)\, dx \tag{B.1.7}$$

and its inverse as

$$\mathcal{F}_\varepsilon^{-1} v(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} e^{-\frac{\mathrm{i}}{\varepsilon}\langle x,\xi\rangle} v(\xi)\, d\xi \tag{B.1.8}$$

We recall here some properties of the semiclassical Fourier transform that will be useful in the following.

Proposition B.1.3. *We have*

$$(\varepsilon D)^\alpha \mathcal{F}_\varepsilon u = \mathcal{F}_h((-x)^\alpha u) \tag{B.1.9}$$

$$\mathcal{F}_\varepsilon((\varepsilon D_x)^\alpha u) = \xi^\alpha \mathcal{F}_\varepsilon u \tag{B.1.10}$$

$$\|u\|_{L^2} = \frac{1}{(2\pi\varepsilon)^{n/2}} \|\mathcal{F}_\varepsilon u\|_{L^2} \tag{B.1.11}$$

Proof. □

Definition B.1.4. *Let $a \in \mathcal{S}(\mathbb{R}^n)$, $a = a(x,\xi)$ be a symbol.*

(i) Weyl quantization

$$a^W(x,\varepsilon D)u(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle} a\left(\frac{x+y}{2},\xi\right) u(y)dyd\xi \tag{B.1.12}$$

(ii) Standard quantization

$$a(x,\varepsilon D)u(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle} a(x,\xi)u(y)dyd\xi \tag{B.1.13}$$

(iii) General quantization

$$Op_t(a)u(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle} a(tx+(1-t)y,\xi)u(y)dyd\xi \tag{B.1.14}$$

Remark B.1.5

(i) It is easy to see that the standard quantization is simply

$$a(x, \varepsilon D)u = \mathcal{F}_\varepsilon^{-1}(a(x, \cdot)\mathcal{F}_\varepsilon u(\cdot))$$

(ii) $\mathrm{Op}_{\frac{1}{2}}(a) = a^W(x, \varepsilon D)$ and $\mathrm{Op}_1(a) = a(x, \varepsilon D)$

The following important theorem is on the composition of pseudodifferential operators. It says that the composition of two PDO is a PDO.

Theorem B.1.6. *Let $a, b \in \mathcal{S}(\mathbb{R}^{2n})$. Then*

$$a^W(x, \varepsilon D)b^W(x, \varepsilon D) = (a\#b)^W(x, \varepsilon D) \tag{B.1.15}$$

where

$$a\#b(x, \xi) = e^{\mathrm{i}\varepsilon A(D)}(a(x, \xi)b(y, \eta))|_{y=x,\eta=\xi} \tag{B.1.16}$$

and

$$A(D) = \frac{1}{2}\omega(D_x, D_\xi, D_y, D_\eta) \tag{B.1.17}$$

Proof. □

B.2 Quantization of symbols and Gårding inequalities

First of all we want to understand how the quantization $\mathrm{Op}_t(a)$ works on various symbols that we will use.

Proposition B.2.1. *(i) If $a(x, \xi) = \xi^\alpha$ then*

$$Op_t(a)u = (\varepsilon D)^\alpha u \tag{B.2.1}$$

for all $t \in [0, 1]$.

(ii) If $a(x, \xi) = a(x)$ then

$$Op_t(a)u = a(x)u \tag{B.2.2}$$

for all $t \in [0, 1]$.

(iii) If $a(x, \xi) = \frac{|\xi|^2}{2} + V(x)$ then

$$Op_t(a)u = \frac{|\varepsilon D|^2}{2}u + V(x)u = -\frac{\varepsilon^2}{2}\Delta u + V(x)u \tag{B.2.3}$$

for all $0 \le t \le 1$.

Proof. (i) follows immediately from the definition. (ii) comes from the fact that

$$\mathrm{Op}_1(a) = a(x, \varepsilon D) = a(x)$$

Then we compute

$$\begin{aligned}
\partial_t \mathrm{Op}_t(a)u &= \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle} \langle \partial a(tx + (1-t)y)|x-y\rangle u(y) dy d\xi \\
&= \frac{\varepsilon}{\mathrm{i}(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \mathrm{div}_\xi \left(\int_{\mathbb{R}^n} e^{\frac{\mathrm{i}}{\varepsilon}\langle x-y|\xi\rangle} \partial a(tx + (1-t)y) u(y) dy \right) d\xi \\
&= \frac{\varepsilon}{\mathrm{i}(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \mathrm{div}_\xi \left(e^{\frac{\mathrm{i}}{\varepsilon}\langle x|\xi\rangle} \widehat{\alpha}(\xi) \right) d\xi
\end{aligned}$$

where we have posed $\alpha(y) = \partial a(tx + (1-t)y)u(y)$. Since $a \in \mathcal{S}(\mathbb{R}^n)$ then $\widehat{\alpha}(\xi) \to 0$ as $|\xi| \to \infty$ and the last expression is zero. Then for all $0 \le t \le 1$ we have $\mathrm{Op}_t(a)u = \mathrm{Op}_1(a)u = au$. (iii) is obtained using (i) and (ii). ☐

B.3 Quantization on the torus

First of all we identify the n-dimensional torus with the set

$$\mathbb{T}^n = \{x \in \mathbb{R}^n | 0 \le x_i < 1, \;\; 1 \le i \le n\}$$

and we consider as function on $\mathbb{T}^n$ the pertiodic functions on $\mathbb{R}^n$:

$$u(x + k) = u(x)$$

where $k \in \mathbb{Z}^n$. Then, moving to the symbols, we identify a symbol on $\mathbb{T}^n \times \mathbb{R}^n$ with symbols on $\mathbb{R}^n \times \mathbb{R}^n$ that are periodic in x:

$$a(x + k, \xi) = a(x, \xi)$$

where $k \in \mathbb{Z}^n$. If we quantize such a symbol then we get

$$(a^W(x, \varepsilon D)u)(x + k) = (a^W(x, \varepsilon D)u(\cdot + k))(x)$$

so these operators preserve periodicity.

B.4 Defect measures

We consider a bounded sequence $\{u(\varepsilon)\}_{0<\varepsilon\le\varepsilon_0}$ in $L^2(\mathbb{R}^n)$, that is

$$\sup_{0<\varepsilon\le\varepsilon_0} \|u(\varepsilon)\|_{L^2} < \infty$$

The first important theorem of this section gives us a bound for the norm of a Weyl quantized operator.

Theorem B.4.1. *Suppose that $a \in \mathcal{S}(\mathbb{R}^n)$. Then*

$$\|a^W(x, \varepsilon D)\|_{L^2 \to L^2} \leq C \sup_{\mathbb{R}^{2n}} |a| + O(\sqrt{\varepsilon}) \tag{B.4.1}$$

Proof. □

The next theorem implies the existence of the so called microlocal defect measures.

Theorem B.4.2. *There exists a Radon measure μ on $\mathbb{R}^{2n}$ and a sequence $\varepsilon_j \to 0$ such that*

$$\langle a^W(x, \varepsilon D) u(\varepsilon_j) | u(\varepsilon_j) \rangle \to \int_{\mathbb{R}^{2n}} a(x, \xi) d\mu \tag{B.4.2}$$

for every symbol $a \in C_c^\infty(\mathbb{R}^{2n})$.

Proof. We choose a sequence $\{a_k\}_{k=0}^\infty \subset C_c^\infty(\mathbb{R}^{2n})$ that is dense in $C_c(\mathbb{R}^{2n})$. Then we select $\varepsilon_j^1 \to 0$ such that

$$\langle a_1^W(x, \varepsilon_j^1 D) u(\varepsilon_j^1) | u(\varepsilon_j^1) \rangle \to \alpha_1$$

Now we choose a subsequence $\{\varepsilon_j^2\} \subset \{\varepsilon_j^1\}$ such that

$$\langle a_2^W(x, \varepsilon_j^2 D) u(\varepsilon_j^2) | u(\varepsilon_j^2) \rangle \to \alpha_2$$

and going further in this way, we use a standard diagonal argumet to get a sequence $\{\varepsilon_j\}$, where $\varepsilon_j = \varepsilon_j^j \to 0$, such that

$$\langle a_k^W(x, \varepsilon_j D) u(\varepsilon_j) | u(\varepsilon_j) \rangle \to \alpha_k$$

for all k. We define $\Phi(a_k) := \alpha_k$. Then for every k we have

$$|\Phi(a_k)| = |\alpha_k| = \lim_{\varepsilon_j \to 0} |\langle a_k^W(x, \varepsilon_j D) u(\varepsilon_j) | u(\varepsilon_j) \rangle| \leq C \limsup_{\varepsilon_j \to 0} \|a_k^w\| \leq C \sup_{\mathbb{R}^{2n}} |a_k|$$

So Φ is defined on a dense subset of $C_c(\mathbb{R}^{2n})$, is linear and bounded: we can extend it to a bounded linear functional on $C_c(\mathbb{R}^{2n})$ and it holds

$$|\Phi(a)| \leq C \sup_{\mathbb{R}^{2n}} |a|$$

for all $a \in C_c(\mathbb{R}^{2n})$. The last step is to apply Riesz representation Theorem that implies the existence of a complex valued Radon measure on $\mathbb{R}^{2n}$ such that

$$\Phi(a) = \int_{\mathbb{R}^{2n}} a(x, \xi)\, d\mu$$

□

Definition B.4.3. *We call μ a microlocal defect measure associated with the family $\{u(\varepsilon)\}_{0<\varepsilon\leq\varepsilon_0}$.*

Theorem B.4.4. *The measure μ is real and non negative, i.e.*

$$\mu \geq 0$$

Proof. We have to show that if $a \geq 0$ than

$$\int_{\mathbb{R}^{2n}} a(x,\xi)\, d\mu \geq 0$$

Now if $a \geq 0$ one has

$$\langle a^W(x,\varepsilon D)u(\varepsilon)|u(\varepsilon)\rangle \geq -C\varepsilon\|u(\varepsilon)\|^2_{L^2}$$

(using the sharp Gårding inequality). Then if we take the limit $\varepsilon \to 0$ we have

$$\int_{\mathbb{R}^{2n}} a(x,\xi)\, d\mu = \lim_{\varepsilon\to 0}\langle a^W(x,\varepsilon D)u(\varepsilon)|u(\varepsilon)\rangle \geq 0$$

as required. $\square$

Example B.4.5. The following example is about stationary phase and defect measures. We consider

$$u(\varepsilon;x) = b(x)e^{\frac{i}{\varepsilon}\varphi(x)}$$

where we suppose $\varphi, b \in C^\infty$ and $\|b\|_{L^2} = 1$. For $\varepsilon \to 0$ we have

$$\langle a^W(x,\varepsilon D)u(\varepsilon;x)|u(\varepsilon;x)\rangle \to \int_{\mathbb{R}^n} a(x,\partial\varphi(x))|b(x)|^2dx = \int_{\mathbb{R}^n} a(x,\xi)d\mu$$

once we choose $\mu = |b(x)|^2\delta_{\{\xi=\partial\varphi(x)\}}\mathcal{L}^n$.

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