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Semiclassical analysis of the Schrödinger equation with singular potentials

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Abstract

In the first part of this thesis we study the propagation of Wigner measures linked to solutions of the Schrödinger equation with potentials presenting conical singularities and show that they are transported by two different Hamiltonian flows, one over the bundle cotangent to the singular set and the other elsewhere in the phase space, up to a transference phenomenon between these two regimes that may arise whenever trajectories in the outsider flow lead in or out the bundle. We describe in detail either the flow and the mass concentration around and on the singular set and illustrate with examples some issues raised by the lack of unicity for the classical trajectories on the singularities despite the unicity for quantum solutions, dismissing any classical selection principle, but in some cases being able to fully solve the problem.

In the second part we present a work in collaboration with Dr. Clotilde Fermanian and Dr. Fabricio Macià where we analyse a Schrödinger-like equation pertinent to the semiclassical study of the dynamics of an electron in a crystal with impurities, showing that in the limit where the characteristic length of the crystal's lattice can be considered sufficiently small with respect to the variation of the exterior potential modelling the impurities, then this equation is approximated by an effective mass equation, or, more generally, that its solution decomposes in terms of Bloch modes, all of them satisfying effective mass equations specifically assigned to their Bloch energies.

Résumé

Dans la première partie de cette thèse nous étudions la propagation des mesures de Wigner associées aux solutions de l'équation de Schrödinger à potentiels présentant des singularités coniques, et nous montrons qu'elles sont transportées par deux différents flots Hamiltoniens, l'un sur le fibré cotangent à la variété des singularités et l'autre ailleurs dans l'espace des phases, à moins d'un phénomène d'échange entre ces deux régimes qui peut se produire quand des trajectoires du flot extérieur atteignent le fibré cotangent. Nous décrivons en détail et le flot et la concentration de masse autour et sur la variété singulière, et illustrons avec des exemples quelques questions issues de la faute d'unicité des trajectoires classiques sur les singularités en dépit de l'unicité des solutions quantiques, ce qui refute tout principe de sélection classique, mais qui n'empêche dans certains cas de résoudre complètement le problème.

Dans la deuxième partie nous présentons un travail mené en collaboration avec Dr. Clotilde Fermanian et Dr. Fabricio Macià où nous analysons une équation de type Schrödinger pertinente à l'étude semiclassique de la dynamique d'un électron dans un cristal avec impuretés et montrons que, dans la limite où la période caractérisique du réseau cristallin est sufisamment petite par rapport à la variation du potentiel extérieur représentant les impuretés, cette équation peut être approximée par une équation de masse effective, ou, plus généralement, que sa solution se décompose en modes de Bloch et que chacun d'eux satisfait une équation de masse effective spécifique à son énergie de Bloch.

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Acknowledgements

Why should people use “we” instead of “I” in scientific communication is a matter that was explaining Profª Cida, a teacher of mine back in High School, more than a decade ago. An issue of impersonality. Not of course in the sense of denying your own participation in the scientific progress, what would be rather a nonsense than a proper sense; not in the aim of making things appear like no human was behind the text as in a user’s guide or so, on the contrary as we’ll see. In fact, the actual reason is such, that only with time, work and growth I could get to fully understand.

It’s something that another Victor glimpsed when naming neither his prisoner condemned to death nor the crime he was convicted of as a manner to extend his fierce campaign against the capital penalty to the universality of men and faults. It’s an expedient which nowhere as in the insistent anonymity throughout *Les Misérables* has someone driven so deep as this Victor, who opened room in his romance to each miserable in the world by making them recognizable under some of the many anonymous masks that his particular characters wear, of those the protagonist’s one is simply *gens*[1].

It’s an expression of universality through anonymity that is taken to its maximal power in a bishop Myriel’s thought, himself nicknamed Bienvenu:

Oh you who are! The Ecclesiastes name you Almighty, the Maccabees name you Creator, the Epistle to the Ephesians call you Freedom, Baruch name you Immensity, the Psalms name you Wisdom and Truth, John name you Light, the Kings name you Lord, the Exodus call you Providence, Leviticus Holiness, Ezra Justice, the creation name you God, man name you Father; [...] Solomon name you Mercy, and there is the most beautiful of all your names.

Because It is the most universal, no precise nor unique denomination can It be given, for a unique and precise description circumscribes. Whenever possible, whence, the third person “one” is preferable over “we”, said my teacher.

Thus, how could I dare label with my particular identity Victor, of which “I” is only a textual avatar, the universality of teachers, masters, colleagues, scholars, technicians and savants that preceded me and of whose contribution consists all but an atomic portion of this present work, not considering the errors and mistakes ahead, that I claim of my exclusive authorship?

Each time that I chose “we” instead of “I” in this monograph, it’s a tribute that I pay to the very concept of University, this circle encrusted in the middle of our campus in São Paulo whose centre is everywhere, and which, by corollary, includes we all, as an everywhere centred circle must have infinite radius. Hence my reticence in listing the names of those that I can remember who somehow collaborated to this thesis, what wouldn’t be

[1] *Jean Tréjean* in the first manuscripts, or, spoken, *gens très gens*.

more than a partial acknowledgement for their "universitarian", disinterested though crucial contributions, further to being a tremendous injustice to those within this huge circle who also cooperated in their own ways and whom my memory isn't now able to reach.

I only don't hesitate in mentioning here Clotilde Fermanian as one of those I owe more. Although the student appears alone as the author, a good thesis is a project led by two. In addition, she is responsible for pushing Profª Cida's teachings to a concrete learning and for the understanding this carried, through the much work that we've done together and the scientific growth I underwent thanks to her advise, professional exigence and academic example.

And of course Fabricio Macià, whom I had the pleasure to work with and to learn from, and whose smart guesses are deeply imprinted in the following pages. For, along with Clotilde, we shared contributions to many parts of this thesis, confirming once again the misleading character of individual authorship in scientific work.

Therefore, not to be unfair towards all the others, I beg the reader, every time that you find "we" in the following pages, to believe that it's not a simple convention of style, but solely the plural pronoun "we" with its old meaning: it's us, me and my teachers, from Deolinda to Clotilde, who added to my education and guided me from the more general interests to the more technical issues; it's us, me and the great minds whose work is so fundamental that their names are still attached to their inventions, Liouville, Schrödinger, Wigner, others, and based on which I've been working during the last years; it's us, me and the more recent authors who are listed in the bibliography and who allowed me an up-to-date view over the field I'm labouring on; it's me and the personal of LAMA, my fellow PhD students and all the other members of the department; it's me and those who financed my daily needs, the doctoral school MSTIC and all my former funders.

It's me and my friends, who stood at my side and in my company – even if only through a screen – as much time as good and many they are, and since they're really good and many, that was a gorgeous amount of moments ~~not working~~ of joy.

Finally, I do not forget that "we" is me and my family. They who are, (even) if unwittingly, my teachers, my supervisors, my financiers, my police, my headaches, my doctors, my progenitors, my deads, my grieves, my nurses, my contenders, my counsellors, my judges, my advisors, my supporters, my opponents, my annoyances, my friends, my competitors, my partners.

My upbringing. My uprisings...

Oh you who are!

Part I

Introduction

Chapter 1

General Introduction

A key problem in mathematics and in its applications is to study how solutions to partial differential equations (field equations) with a given parameter (a coefficient of thermal diffusion, the speed of wave propagation in some medium, the mass of a quantum particle, *et cætera*) tend to some significant limit function or distribution as this parameter becomes too big or too small.

Of course there are much to be made precise about the above statement: how much regularity do we require for the solutions of the equations? how this regularity may be lost as the parameter becomes too big or too small? in which sense the limits of these solutions are to be understood? how will they behave as time passes?

The techniques developed in addressing these questions, as well as the many answers they have been allowing us to get, form the corpus of *Semiclassical Analysis*. Although in the present work we restricted ourselves to the study of Schrödinger-like equations with rough potentials[1], the scope of uses one can make of it in many different fields of Mathematics, Physics and other so-called exact sciences is far broader.

In the next introductory sections we hope to give the reader an idea of the richness of Semiclassical Analysis by looking at the problems that motivated some of its most important objects, usually variants or refinements of the grounding concept of *defect measure* – a measure that seeks to quantify the "lack of compacity", the "lack of convergence" of a sequence of functions. But previously, we will present our own personal view of this theory, which – given my backgrounds – could not be unrelated to the matter of re-obtaining the classical XVIIIth to XIXth century Mechanics from the quantum Mechanics developed in the first decades of the last century and now largely accepted, if not as an ultimate theory, surely as the suitable paradigmatic basis for our understanding of physics.

For the convenience of the non-specialist reader, the hardcore mathematics will not start before next chapter. This one is wholeheartedly devoted to the lay public, especially Section 1.1, that I wrote keeping my engineer friends in mind. Still, we have given a lot of interesting bibliographical references in there, so maybe even the specialist reader might enjoy it.

A proper introduction to the specific subjects treated in this work can be found in Chapters 3 and 8.

[1]More precisely, at the first half of the thesis we approach potentials with a particularly impertinent kind of anomalous derivatives, called conical potentials, and at the second one we look at periodic potentials with impurities, a work done in collaboration with Dr. Clotilde Fermanian and Dr. Fabricio Macià.

1.1 The classical limit of Quantum Mechanics

Mechanics is the central theory in physics, be it classical or quantum. Its primacy comes from the fact that its concepts are the basis over which all the others are built: time, position, momentum and determinism in its classical version; time, position and momentum densities and probability in its quantum one. We could vaguely say that the other theories only add to the knowledge of the specific dynamics of their particular systems, and then their kinetics is completely mechanical.

For instance, it is like we said that electromagnetism only gives the specific equation electromagnetic fields obey to and the specific law of force for a particle submitted to them, and therefore we just do Mechanics with this information, *i.e.*, we solve the field and the motion equations dressed in their specific electomagnetic form and obtain quantities like momenta, positions, frequencies, forces and so on as functions of time. Let position, momentum, force, *etc.*, make no longer sense, and classical electromagnetism becomes meaningless.

This is why the way we understand the world ought to rely on the mechanical theory we have in hand. Kinetics, or the description of motion, furnishes thus the paradigm for the subsequent physics to be fashioned by the manner we look at and describe the phenomena around us.

Philosophers and mathematicians in the late XVIIth century looked at nature with deterministic eyes, backed by rationalist (most of the time), investigative minds and deprived of any useful tool to explore the microscopic scale.

Let us shortly list what they saw and thought and how it shaped Classical Mechanics:

1. Things move over time; this remark took them to describe the motion parametrized exclusively and unequivocally by the time variable.

2. It is not enough to say where some thing is in order to say where it will be in the future, we need to say in addition in which way its position is changing (momentum); this led to the description of motion departing from two quantities, initial position and momentum, which later developed into the notion of trajectories over a phase space.

3. There must be a natural law governing the motion; it was by Newton realized that this law actually correlates a force acting on a particle with the rate of change of its momentum (acceleration).

In Newton's formulation, the motion is thus encoded by the quantity "position as function of time", $x(t)$, and is ruled by what in modern mathematics we call a differential equation of second order:

$$\frac{d^2}{dt^2}x(t) = F(t, x(t), \xi(t)).$$

The forces in general may depend on time t, position x and momentum ξ, in agreement with Item 2. However, to make things simpler, let us suppose that the force only depends on the position[2], $F = F(x)$, in which case it is more reasonable to thing of the force as a property of the space itself. In other words, $F(x) = -\nabla V(x)$, where V is a potential spread over the space and has nothing to do with the moving particles.

[2]If it depends on t, nothing especial changes, and if it depends on ξ as well, then we will have unnecessary technical difficulties, the central ideas remaining the same.

Then, remembering that momentum is essentially the rate of change in position, Newton's equations can be written as a pair of first order equations:

$$\begin{cases} \frac{d}{dt}x(t) = \xi(t) \\ \frac{d}{dt}\xi(t) = -\nabla V(x(t)), \end{cases}$$

which are the Hamilton's equations. This is already good because solving first order equations is easier than second order, but Hamilton's smartness eventually went further: he realized that writing down the expression for the energy[3] of a particle as a function of x and ξ,

$$H(x,\xi) = \frac{1}{2}\xi^2 + V(x),$$

the motion equations become:

$$\begin{cases} \frac{d}{dt}x(t) = \partial_\xi H(x(t),\xi(t)) \\ \frac{d}{dt}\xi(t) = -\partial_x H(x(t),\xi(t)). \end{cases}$$

Geometrically, this has an immediate interpretation: the solutions $(x(t),\xi(t))$ of this system are the trajectories of the flow induced by the vector field $(\partial_\xi H(x,\xi), -\partial_x H(x,\xi))$ over the plane $O_{x\xi}$, called phase space. The precise trajectory a particle will take in this flow is decided by its initial state represented by a point $(x(0),\xi(0))$, when intervenes a theorem of unicity saying that if V is not much irregular, then through any point of the phase space there will be only one trajectory passing.

For our purposes, what is to be retained from this brief explanation is that, now, if we are able to define any quantity we want to measure in a particle's motion as a function over the phase space, say $Q = Q(x,\xi)$, then the only thing we need to do in order to know how this quantity varies with time is to calculate the Hamiltonian trajectory for the particle and then compose Q with it, $Q(t) = Q(x(t),\xi(t))$.

Now, for Quantum Mechanics, the picture is more complicated.

There has been a huge hysteria, even in serious scientific literature, about the strangeness and the ununderstandability of Quantum Mechanics. Apparently, just because Feynman declared that *safely nobody understands Quantum Mechanics*[48], we are destined never to understand it, even if fortunately he also said that *you know how it always is, every new idea, it takes a generation or two until it becomes obvious that there's no real problem*[47].

We do not mean that Quantum Mechanics epistemological implications are fully understood; if they are, it is not to our current knowledge. Nonetheless, if Classical Mechanics implications were ever fully accepted, this is not to our current knowledge neither[4].

[3]As a technical remark, the Hamiltonian function H is not always the energy as we wrote (nor is the momentum). The reader willing to go deeper into the details is referred to [72].

[4]Newton himself was upset that his theory relied on such absurd an assumption as a gravitational force that instantly propagates through the space:

"Tis inconceivable that inanimate brute matter should (without the mediation of something else which is not material) operate upon & affect other matter without mutual contact; as it must if gravitation in the sense of Epicurus be essential & inherent in it. And this is one reason why I desired you would not ascribe innate gravity to me. That gravity should be innate inherent & essential to matter so that one body may act upon another at a distance through a vacuum without the mediation of any thing else by & through which their action or force may be conveyed from one to another is to me so great an absurdity that I believe no man who has in philosophical matters any competent faculty of thinking can ever fall into it."[89]

Classical Mechanics offers a weird universe of imprisonment, whereas Quantum Mechanics brings us something that may still appear not completely sensible (although there has been a lot of progress since Feynman), but which is much closer to the impredictable world that we really and freely live in. Besides, it is now known that the quantum postulates result from a set of axioms that, so as to say, correspond to the way we think the world should be (causality, state distinguishability, etc.)[33, 62], which, in Scott Aaronson's words, is by and large a generalized theory of probability allowing for non-positive distributions[1].

Even the dynamical content of Quantum Mechanics, albeit known not to be ultimately accurate[5], can be guessed from a careful analysis of experimental data (in [95] it is discussed how the rates of decay between different levels in the hydrogen spectrum led to a matricial theory ruled by the Heisenberg equation), so, as we see, there is no point in stressing how strange or elusive Quantum Mechanics is.

This said, let us present some of Quantum Mechanics without going deep into the interpretative details.

Here, the state of a particle is described by a L^2 function, *i.e.*, a function Ψ of the positions x such that $|\Psi|^2$ is integrable and stands for the distribution of probability of finding this particle in the different regions of the space[6]. Since the probability of finding the particle somewhere is 1, then $\int |\Psi(x)|^2\, dx = 1$. We cannot, however, drop Ψ down and rely only on $|\Psi|^2$, for the distribution of probability of measuring the particle within a certain range of momenta is given from the Fourier transform $\hat{\Psi}$, through the same procedure of taking its square module $|\hat{\Psi}|^2$ and integrating it with respect to the momenta ξ.

Naturally, this implies that the particle cannot be found exactly on a point (x, ξ), as more precision in a position measurement carries a greater variance in the momenta one and vice-versa. This is called the *uncertainty principle* and is completely analogous – at least mathematically – to the statement in Signal Analysis (engineering stuff) that says that the shorter a pulse in time, the broader the range of frequencies that must be superposed to generate it. This fact undermines any hope to study the trajectory of a particle in the phase space, which was the core of Classical Mechanics. Trajectory, in the quantum framework, makes just no sense.

In spite of that, nowadays the classical theories are presented to us as the "intuitive" ones, in opposition to the mysterious quantum world of EPR paradox (which, by the way, Information Theory makes sense of[3]). Besides, Classical Mechanics radical determinism implied that the future must had been already written, for the state of the universe in a precise instant would be completely defined and, as we said, from one point in the phase space departs only a unique trajectory.

It should be highly striking that, in the rational XIXth century, clairvoyance was only forbidden by shortage of technical resources: too much data to analyse if one wants to predict his own future. Of course we could lift the tacit assumption that our potentials are smooth and so the trajectories are uniquely defined, but this implies either that Classical Mechanics is not a theory, since it would give no useful answers, or that it needs some selection principles or probabilistic add-ons so we could know how different trajectories are chosen in case of non-unicity. Yet, is it not the probabilistic features of Quantum Mechanics and its exclusion principle two of its aspects of more outspoken strangeness?

For more on this topic, see Chapter 3, where we analyse the possibility of inducing selection principles in Classical Mechanics from the quantum theory.

[5] Hence the many field theories that have been proposed since the very beginning of Quantum Mechanics, when Schrödinger discarded the Klein-Gordon equation he had first obtained for it described a completely wrong fine structure for the hydrogen's spectrum (which is understandable, since Klein-Godon only applies for spinless particles and the hydrigen's electron has half-integer spin)[53].

[6] In [28] Ψ is a state of knowledge about the particle rather than an attribute of the particle itself, in a somewhat Bayesian approach.

The way the theory predicts the possible outputs for measuring some physical quantity of a particle is through a special class of operators, called self-adjoint, that act on the functions Ψ. So, if to some classical quantity Q (the angular momentum for instance) we have associated the operator $\hat{Q}$, then the average $\langle \hat{Q} \rangle$ of the values we can get in measuring particles in the state Ψ is given by:

$$\left\langle \hat{Q} \right\rangle = \left\langle \hat{Q}\Psi \, , \Psi \right\rangle ,$$

where the notation $\langle \Psi_1 \, , \Psi_2 \rangle$ is simply a shortcut for the inner product $\int \Psi_1(x)\overline{\Psi_2(x)}dx$.

What about the precise values we can get? Well, this is a bit more delicate; we would need to talk about the spectrum of $\hat{Q}$ and its spectral decomposition[7]. It is from the average $\langle \hat{Q} \rangle$ that we will recover the classical measurement for Q on the phase space in the semi-classical limit, thus it is with these averages that we will work in this thesis. Note, however, that every time that we perform an actual measurement we change radically the state of the particle (or of our knowledge about it, as in [28]), so unlike in the classical theory, here the interaction between the observed particle and the observer is crucial for the system's evolution[36, 50, 109].

Furthermore, a particle of mass $m = 1$ initially in a state Ψ_0, if remaining not observed, evolves under a potential V to a state Ψ_t which is solution to the Schrödinger equation:

$$i\hbar\partial_t \Psi_t(x) = -\frac{\hbar^2}{2}\Delta\Psi_t(x) + V(x)\Psi_t(x),$$

where Δ is the Laplacian operator and $\hbar$ is the Planck's constant. We could have written $i\hbar\partial_t\Psi_t(x) = \hat{H}\Psi_t(x)$, where the operator

$$\hat{H} = -\frac{\hbar^2}{2}\Delta\Psi_t(x) + V(x),$$

called *Hamiltonian*, is closely related to the classical Hamiltonian function introduced above.

In short, the quantum programme is: take an initial state, evolve it inside the Schrödinger equation, measure it using the inner product and destroying the state you are measuring. Let us compare the quantum and the classical theories:

	Classical Mechanics	**Quantum Mechanics**
Description	phase space deterministic	Hilbert space (L^2) probabilistic
Dynamics	trajectories Hamilton's equations	uncertainty principle Schrödinger's equation
Measurement	composition with trajectories preserves the measured state	inner product destroys the measured state

It is widely accepted that the classical should follow from the quantum in the limit where the Planck's constant $\hbar$ tends to zero. The uncertainty principle, for example, establishes a relation between the variances of measurements of position and momentum which is minimized by a factor $\hbar$, so, if it goes to 0, we could wishfully speak of states precisely localized at a point (x, ξ) of the phase space.

[7] See [60] for an introductory course on Quantum Mechanics and [39, 100] for more complete texts. For a mathematical formalization of the concepts treated in these references, see [88].

There are other heuristic reasons to believe that the classical limit emerges with $\hbar$ tending to 0: in the introduction of our Master's degree monograph[29], we repeated an argument saying that this limit would imply a recover of a classical trajectory-like theory from a quantum undullatory one according to the scheme of the opto-mechanics approximation[8], but this reasoning could not be made rigorous since not all the possible solutions of the Schrödinger equation can be written under the necessary *Ansatz*. Several other methods for recovering the classical theory were proposed, always taking (not very careful) limits $\hbar \longrightarrow 0$, as did Bohr[9] and De Broglie[10].

The first method at least teaches us something about Optics.

Anyway, the heuristics is convincing and we will consider both the Hamiltonian operator and the quantum states as parametrized by the Planck's constant, so the Schrödinger equation reads $i\hbar\partial_t \Psi_t^\hbar(x) = \hat{H}^\hbar \Psi_t^\hbar(x)$, *i.e.*, a partial differential equation with a parameter to be taken small.

Now, the first thing to do is to look for a function that could join the information about the distributions in x and in ξ contained respectively in $\Psi^\hbar$ and $\hat{\Psi}^\hbar$. This is the *$\hbar$-Wigner transform*:

$$W^\hbar \Psi_t^\hbar(x,\xi) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar}\xi \cdot y} \Psi_t^\hbar \left(x - \frac{y}{2}\right) \overline{\Psi_t^\hbar \left(x + \frac{y}{2}\right)} dy.$$

This transform, although not itself a distribution of probability over the phase space (for it is not necessarily positive), is already a function of x and ξ, so we are back from the Hilbert to the phase space. Moreover, its marginal integrals are indeed probability distributions, those we wanted to get:

$$\int W^\hbar \Psi_t^\hbar(x,\xi) d\xi = \left|\Psi_t^\hbar(x)\right|^2 \qquad \text{and} \qquad \int W^\hbar \Psi_t^\hbar(x,\xi) dx = \frac{1}{\varepsilon^d} \left|\hat{\Psi}_t^\hbar \left(\frac{\xi}{\varepsilon}\right)\right|^2.$$

Moreover, the Wigner transforms obey to some equations that are similar up to an error of order ε to those satisfied by the classical continuous distributions of mass, like the equation of continuity in phase and in position spaces and the Liouville equation[75] (which is just the form that Hamilton's equations assume for functions of x and ξ).

As a first remark, the Wigner transforms may already be used as a vehicle for moving from quantum to classical, upon to a proper definition of convergence when $\hbar \longrightarrow 0$. This could be the standard limit of some sequence extracted from integrals such as $\int W^\hbar \Psi_t^\hbar(x,\xi) Q(x,\xi) dx d\xi$, where Q is the ancient classical observable over the phase space. This is a sensible notion of limit, since if $W^\hbar \Psi_t^\hbar$ were a classical distribution of mass, then these integrals would give the correspondent average measurements of the quantity Q.

---

[8]The principle that says – and which is mathematically verified – that light waves with sufficiently small wavelengths with respect to the distances they travel and the size of the objects they interact with (reflecting, refracting, *etc.*) can be considered as light rays following the trajectories one would expect a classical particle to do.

[9]The gap between two possible values for the energy of an electron in a linked state is proportional to $\hbar$, thus as classically its energies would be expected to form a continuous range, one would need have $\hbar$ tending to 0 in order to recover the classical theory[40].

[10]The matter has oscillatory properties and the wavelengths of macroscopic matter (which are proportional to $\hbar$) are very small, since it is highly localized in space[40].

More precisely, we will say that $W^\hbar\Psi_t^\hbar$ converges to μ_t as $\hbar$ tends to 0 if there is some sequence $\hbar_n$ going to zero such that for any (reasonable) Q on the phase space we have[11]

$$\int W^{\hbar_n}\Psi_t^{\hbar_n}(x,\xi)Q(x,\xi)dxd\xi \underset{n\to\infty}{\longrightarrow} \int Q(x,\xi)d\mu_t(x,\xi),$$

and this time μ_t is a true positive distribution of probability on $O_{x\xi}$, called a *Wigner measure*[12] for the concentration of the family $\left(\Psi_t^\hbar\right)_{\varepsilon>0}$. As expected, μ_t satisfies the same equations as distributions of mass, like continuity in space, in phase space and Liouville[75].

A second remark is that these distributions of mass are much better understood under the formalism of Statistical Mechanics than of mechanics of continuous media (because it is strange to talk about different pieces of mass occupying the same place in space, the same x, but having different momenta ξ). The limits μ_t offer a much richer picture than the usual one-particle description presented in the beginning of this section, what is however a particular case of semiclassical concentration, where the quantum states $\Psi_t^\hbar$ are such that the corresponding μ_t reduces to a Dirac mass on a specific point (x,ξ).

Colloquially, to say that μ_t satisfies a Liouville equation means that it is transported, carried by the classical Hamiltonian flow over the phase space, so if we have a measure μ_0 initially concentrated to the point (x_0,ξ_0), it means that μ_t will be at the point $(x(t),\xi(t))$, following the unique trajectory given by Hamilton's equations that passes by (x_0,ξ_0) at $t=0$. This is the particular case of concentration where one can fairly think of μ_t as a particle moving as it is predicted in Classical Mechanics.

In Chapter 2 we will review these facts with rigorous technical concerns. Then, in Section 3.1 we will consider a case where the classical flow is ill-defined, this is to say, where thanks to irregularities in the potential the trajectories may split on some points, even though the quantum solutions to the Schrödinger equation remain unique. There, it is going to be important to know with precision under which conditions the affirmations stated in the paragraphs above do hold, and in which mathematical sense.

As a last comment, for the quantum operators $\hat{Q}^\hbar$ whose expressions are explicitly known, such as the Hamiltonian $\hat{H}^\hbar$, the position $\hat{x}^\hbar = x$, the momentum $\hat{\xi}^\hbar = -\hbar\nabla$ and its derivates, a short calculation shows that:

$$\left\langle \hat{Q}^\hbar\Psi_t^\hbar, \Psi_t^\hbar \right\rangle = \int W^\hbar\Psi_t^\hbar(x,\xi)Q(x,\xi)dxd\xi,$$

where Q is the classical quantity that corresponds to $\hat{Q}^\hbar$. From this identity we can try to define quantum operators reversely from a classical observable, which leads, after another short calculation, to the *Weyl quantization* formula:

$$\hat{Q}^\hbar\Psi(x) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\xi\cdot(x-y)}Q\left(\frac{x+y}{2},\xi\right)\Psi(y)dyd\xi,$$

providing us with (essentially) self-adjoint operators[38] on the L^2 functions Ψ whenever Q is a real function.

[11] This notion of limit, where we are rather interested in the limits of $W^\hbar\Psi_t^\hbar$ integrated against some function instead of the limits of $W^\hbar\Psi_t^\hbar$ itself (uniform or puntcual), is called *weak convergence*, and it is the more adequate regarding probability distributions, since we are a lot more worried about the averages and variances they give than about what happens to them alone.

[12] It may of course not be necessarily unique, for its derivation depends on the particular sequence $\hbar$ we chose.

The objects resulting from this procedure are called *$\hbar$-pseudodifferential operators* and can be considered as a generalization of the common differential operators (which are the same thing as defined above, but with Q constrained to be a polynomial in ξ)[29]. They are a central tool in Semiclassical Analysis, which is why in the next section we start our formal study by reviewing their most relevant properties.

Chapter 2

Semiclassical Analysis

2.1 Symbolic calculus

Let us consider the ε-pseudodifferential operators $\mathrm{op}_\varepsilon(a) \in \mathcal{L}\left(L^2(\mathbb{R}^d)\right)$ of symbols $a \in C_0^\infty\left(\mathbb{R}^{2d}\right)$ given by the formula:

$$\text{(2.1.1)} \qquad \mathrm{op}_\varepsilon(a)\,\Psi(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-y)} a\left(\frac{x+y}{2},\xi\right)\Psi(y)\,d\xi dy \quad \text{for } \Psi \in L^2(\mathbb{R}^d),$$

which provides self-adjoint operators for real-valued symbols[38]. Of central importance is the fact that they are uniformly bounded in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$ with respect to ε ([9, 38]): there exist constants $K, \tilde{K} > 0$ such that

$$\text{(2.1.2)} \qquad \|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \leqslant K \sup_{\substack{\alpha\in\mathbb{N}_0^d\\ |\alpha|\leqslant d+1}} \sup_{\xi\in\mathbb{R}^d}\int_{\mathbb{R}^d}\left|\partial_x^\alpha a(x,\xi)\right| dx,$$

or, else,

$$\text{(2.1.3)} \qquad \|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \leqslant \tilde{K} \sup_{\substack{\alpha\in\mathbb{N}_0^d\\ |\alpha|\leqslant d+1}} \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}\left|\partial_\xi^\alpha a(x,\xi)\right| d\xi.$$

Remark 2.1.1. Inequalities (2.1.2) and (2.1.3) give upper bounds for the Schur estimate for the norm of $\mathrm{op}_\varepsilon(a)$. Besides, these formulæ remain valid when one uses different scales of ε in different variables, like for an operator $\mathrm{op}_{\varepsilon^\alpha,\varepsilon^\beta}(a) = \mathrm{op}_1(a(x,\varepsilon^\alpha\xi',\varepsilon^\beta\xi''))$, with $\xi = (\xi',\xi'')$ and $\alpha,\beta \geqslant 0$.

Let be $a, b \in C_0^\infty(\mathbb{R}^{2d})$. From equation (2.1.1) it is clear that, for any $\lambda \in \mathbb{C}$, one has

$$\mathrm{op}_\varepsilon(a+\lambda b) = \mathrm{op}_\varepsilon(a) + \lambda\mathrm{op}_\varepsilon(b);$$

besides, noting $\{\ ,\ \}$ the usual Poisson bracket:

$$\text{(2.1.4)} \qquad \mathrm{op}_\varepsilon(\{a\,,b\}) = \frac{i}{\varepsilon}\left[\,\mathrm{op}_\varepsilon(a)\,,\mathrm{op}_\varepsilon(b)\,\right] + \varepsilon R^\varepsilon,$$

with

$$\|R^\varepsilon\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \leqslant \sup_{\substack{\sigma\in\mathbb{N}_0^d\\ |\sigma|\leqslant d+1}} \sup_{\substack{\alpha,\beta\in\mathbb{N}_0^d\\ |\alpha|+|\beta|=2}} \sup_{x\in\mathbb{R}^d}\left\|\partial_x^\alpha\partial_\xi^{\beta+\sigma}a(x,\cdot)\right\|_{L^1(\mathbb{R}^d)}\left\|\partial_x^\beta\partial_\xi^{\alpha+\sigma}b(x,\cdot)\right\|_{L^1(\mathbb{R}^d)}.$$

Remark 2.1.2. When working with smooth and Abelian symbols, one can have a remainder of order ε^2 in (2.1.4). In this thesis, however, we will deal with potentials who fail to be differentiable and whose second derivatives will be unbounded near some singular points, making (2.1.4) and its corresponding error R^ε a suitable formula, even if not the sharpest one.

Nonetheless, formula (2.1.1) can be used for more general symbols, although we may lose boundedness, good properties for symbolic calculation, and be forced to restrict their domains. In particular, for V satisfying the Kato-Rellich conditions, the operator

$$\hat{H}^\varepsilon = \mathrm{op}_\varepsilon \left(\frac{\xi^2}{2} + V(x) \right) \tag{2.1.5}$$

defined with domain $H^2(\mathbb{R}^d)$ is unbounded, although still self-adjoint.

2.2 Wigner transforms and Wigner measures

2.2.1 Establishing definitions

Now, consider a family $(\Psi^\varepsilon)_{\varepsilon>0}$ bounded in $L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^d)\right)$ and define the *Wigner transform* $W^\varepsilon\Psi^\varepsilon \in L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^{2d})\right)$ associated to it:

$$W^\varepsilon\Psi_t^\varepsilon\,(x,\xi) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}y\cdot\xi}\,\Psi_t^\varepsilon\left(x-\frac{y}{2}\right)\overline{\Psi_t^\varepsilon\left(x+\frac{y}{2}\right)}\,dy, \tag{2.2.1}$$

which have interesting properties ([52, 75]), such as

$$\int_{\mathbb{R}^d} W^\varepsilon\Psi_t^\varepsilon(x,\xi)d\xi = |\Psi_t^\varepsilon(x)|^2 \quad \text{and} \quad \int_{\mathbb{R}^d} W^\varepsilon\Psi_t^\varepsilon(x,\xi)dx = \frac{1}{\varepsilon^d}\left|\hat{\Psi}_t^\varepsilon\left(\frac{\xi}{\varepsilon}\right)\right|^2,$$

and the fact that they relate to the pseudodifferential operators by means of the formula:

$$\langle\, \mathrm{op}_\varepsilon\,(a)\,\Psi_t^\varepsilon\,,\, \Psi_t^\varepsilon\,\rangle_{L^2(\mathbb{R}^d)} = \langle\, W^\varepsilon\Psi_t^\varepsilon\,,\, a\,\rangle_{\mathbb{R}^{2d}}\,. \tag{2.2.2}$$

When $\varepsilon \longrightarrow 0$, the Wigner transform converges to a finite and positive measure μ on $\mathbb{R}\times\mathbb{R}^{2d}$ ([55, 58, 75]) in the sense that, given a sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ converging to 0, we can extract a subsequence[1] $(\varepsilon_{n_k})_{k\in\mathbb{N}}$ such that, for all $a \in C_0^\infty(\mathbb{R}_t\times\mathbb{R}^{2d}_{x,\xi})$,

$$\langle\, W^{\varepsilon_{n_k}}\Psi^{\varepsilon_{n_k}}\,,\, a\,\rangle_{\mathbb{R}\times\mathbb{R}^{2d}} \underset{k\to\infty}{\longrightarrow} \int_{\mathbb{R}\times\mathbb{R}^{2d}} a\,d\mu. \tag{2.2.3}$$

This is the *semiclassical* or *Wigner measure* related to the concentration of the sequence $(\Psi^{\varepsilon_{n_k}})_{k\in\mathbb{N}}$.

Again, more regularity implies more good properties. From its very construction, one sees that the Wigner measure is always absolutely continuous with respect to the Lebesgue measure dt, so $d\mu(t,x,\xi) = \mu_t(x,\xi)dt$, where $t \longmapsto \mu_t$ is a $L^\infty\left(\mathbb{R}, \mathcal{D}'(\mathbb{R}^{2d})\right)$ function. Furthermore, if for instance Ψ^ε are solutions to an equation of the form

$$i\varepsilon\partial_t\Psi_t^\varepsilon = \mathrm{op}_\varepsilon(b)\Psi_t^\varepsilon, \tag{2.2.4}$$

[1] Of course μ may depend on the subsequence, this is why we refer to it as *a* semiclassical limit, not necessarily *the* classical one (examples of non-unicity in [75]).

with b smooth, compactly supported and real, then one can show by the Ascoli-Arzelà theorem and equation (2.2.10) ahead that in this case, given $T > 0$, $[-T, T] \ni t \longmapsto \mu_t \in \mathcal{D}'(\mathbb{R}^{2d})$ is continuous and there exists another subsequence $\left(\varepsilon_{n_{k'}}\right)_{k' \in \mathbb{N}}$ such that, for each $t \in [-T, T]$ and $a \in C_0^\infty(\mathbb{R}^{2d})$,

$$\left\langle W^{\varepsilon_{n_{k'}}} \Psi_t^{\varepsilon_{n_{k'}}} \, , \, a \right\rangle_{\mathbb{R}^{2d}} \underset{k' \to \infty}{\longrightarrow} \int_{\mathbb{R}^{2d}} a \, d\mu_t. \tag{2.2.5}$$

Remark 2.2.1. Clearly, for any $t \in \mathbb{R}$ one can extract a subsequence $\varepsilon_{n_k(t)}$ such that $W^{\varepsilon_{n_k(t)}} \Psi_t^{\varepsilon_{n_k(t)}} \rightharpoonup \mu_t$; the point here is that the continuity of $t \longmapsto \mu_t$ implies that, staying within a compact $[-T, T]$, these subsequences may be chosen independently of t.

Remark 2.2.2. If Ψ^ε are solutions to the Schrödinger equation, *i.e.*, (2.2.4) with $\hat{H}^\varepsilon$ defined in (2.1.5) instead of $\mathrm{op}_\varepsilon(b)$, then the continuity of $t \longmapsto \mu_t$ is not assured with all generality, for the term with the commutator in (2.2.10) ahead may not be bounded. Even though, boundedness in there may hold under additional assumptions on V, for instance if $\nabla^2 V$ is bounded. As it will be clear in next section, the central point is to have formula (2.1.4) valid with a proper bounded rest R^ε.

Remark 2.2.3. The quadratic form $\langle \, \mathrm{op}_\varepsilon \, (a) \, \Psi \, , \, \Psi \, \rangle_{L^2(\mathbb{R}^d)}$ gives in Quantum Mechanics the average value for the observable $\mathrm{op}_\varepsilon(a)$ in a system in the quantum state Ψ, exactly as does the integral $\int_{\mathbb{R}^{2d}} a \, d\rho$ in classical Statistical Mechanics for the observable a in a system with mass probability density ρ over the phase space. Besides, equation (2.2.5) carries:

$$\langle \, \mathrm{op}_\varepsilon \, (a) \, \Psi_t^\varepsilon \, , \, \Psi_t^\varepsilon \, \rangle_{L^2(\mathbb{R}^d)} \underset{\varepsilon \to 0}{\longrightarrow} \int_{\mathbb{R}^{2d}} a \, d\mu_t,$$

which allows us to understand the Wigner measures as mass distributions, linking the quantum evolution of Ψ^ε given by the Schrödinger equation with that of its semiclassical limits[2].

Further, if μ_t is the semiclassical measure of Ψ_t^ε along some subsequence ε_k such that $|\Psi_t^{\varepsilon_k}|^2$ converges weakly-$\star$ (in $C_0^\infty(\mathbb{R}^d)$ for instance) towards a measure γ_t on $\mathbb{R}^d$, then one has:

$$\int_{\mathbb{R}^d} \mu_t(\cdot, d\xi) \leq \gamma_t, \tag{2.2.6}$$

the equality holding if and only if the sequence $\Psi_t^{\varepsilon_k}$ is *ε-oscillating*[56, 57, 58], which means:

$$\limsup_{\varepsilon_k \to 0} \int_{\|\xi\| > \frac{R}{\varepsilon_k}} \left| \hat{\Psi}_t^{\varepsilon_k}(\xi) \right|^2 d\xi \underset{R \to \infty}{\longrightarrow} 0. \tag{2.2.7}$$

This also implies that μ_t is a finite measure of total mass bounded by $\sup_{k \in \mathbb{N}} \|\Psi_t^{\varepsilon_k}\|_{L^2(\mathbb{R}^d)}^2$.

[2] From a non-statistical point of view, the classical limit properly speaking would be a particular subsequence (ε_{n_k}) that gives a Dirac mass on a certain point of the phase space, corresponding to a singular particle of mass 1 (classically localized on that point) whose quantum evolution is described by (3.1.2). Although it is always possible to find a sequence of quantum states concentrating to a Dirac mass[55], this is not always the case, since one may have μ continuously spread over the phase space. In any way, the quantum-classical correspondence is better understood statistically ([75, 104]), in which frame the situation with the Dirac mass (or a sum of punctual Dirac deltas with total mass 1) should be seen as a special case of statistical distribution.

2.2.2 Transport phenomena

Taking test functions $\Xi \in C_0^\infty(\mathbb{R})$ and $a \in C_0^\infty(\mathbb{R}^{2d})$ and supposing Ψ^ε solution of (2.2.4), the semiclassical measure μ linked to the family $(\Psi^\varepsilon)_{\varepsilon>0}$ may be given as

$$\langle \mu(t,x,\xi), \Xi(t)\, a(x,\xi) \rangle_{\mathbb{R}\times\mathbb{R}^{2d}} = \operatorname{sc}\lim \int_{\mathbb{R}} \Xi(t) \langle \operatorname{op}_\varepsilon(a)\, \Psi_t^\varepsilon, \Psi_t^\varepsilon \rangle \, dt \tag{2.2.8}$$

(here $\operatorname{sc}\lim$ stands for *semiclassical limit*, abstracting which particular subsequence $(\varepsilon_{n_k})_{k\in\mathbb{N}}$ is to be taken).

From this expression we can evaluate the distribution $\partial_t \mu$:

$$\begin{aligned} \langle \partial_t\mu(t,x,\xi), \Xi(t)\, a(x,\xi) \rangle_{\mathbb{R}\times\mathbb{R}^{2d}} &= -\int_{\mathbb{R}\times\mathbb{R}^{2d}} \Xi'(t)\, a(x,\xi)\; d\mu(t,x,\xi) \\ &= \operatorname{sc}\lim \int_{\mathbb{R}} \Xi(t) \frac{d}{dt} \langle \operatorname{op}_\varepsilon(a)\, \Psi_t^\varepsilon, \Psi_t^\varepsilon \rangle \, dt; \end{aligned} \tag{2.2.9}$$

moreover, in view of (2.2.4) and (2.1.4), we have

$$\begin{aligned} \frac{d}{dt} \langle \operatorname{op}_\varepsilon(a)\, \Psi_t^\varepsilon, \Psi_t^\varepsilon \rangle &= \left\langle \frac{i}{\varepsilon} [\operatorname{op}_\varepsilon(b), \operatorname{op}_\varepsilon(a)]\, \Psi_t^\varepsilon, \Psi_t^\varepsilon \right\rangle \\ &= \operatorname{op}_\varepsilon(\{b, a\}) + \mathcal{O}(\varepsilon). \end{aligned} \tag{2.2.10}$$

Then, putting together (2.2.9) and (2.2.10):

$$\langle \partial_t\mu(t,x,\xi), \Xi(t)\, a(x,\xi) \rangle_{\mathbb{R}\times\mathbb{R}^{2d}} = \langle \mu(t,x,\xi), \Xi(t)\, \{b(x,\xi), a(x,\xi)\} \rangle_{\mathbb{R}\times\mathbb{R}^{2d}}$$

for every test function $\Xi\, a \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, which ultimately induces a differential equation for μ in the sense of the distributions:

$$\partial_t\mu(t,x,\xi) + \{b(t,x,\xi), \mu(x,\xi)\} = 0 \qquad \text{in} \qquad \mathcal{D}'(\mathbb{R}\times\mathbb{R}^{2d}), \tag{2.2.11}$$

or equivalently:

$$\begin{cases} \partial_t\mu_t(x,\xi) + \{b(x,\xi), \mu_t(x,\xi)\} = 0 \\ \mu_{t=0}(x,\xi) = \mu_0(x,\xi) \end{cases} \qquad \text{in} \qquad \mathcal{D}'(\mathbb{R}^{2d}), \tag{2.2.12}$$

where μ_0 is the corresponding semiclassical limit of $W^\varepsilon\Psi_0^\varepsilon$.

These equations may be interpreted as a transport phenomenon that the measure μ undergoes along the flow induced by the vector field $(\partial_\xi b(x,\xi), -\partial_x b(x,\xi))$,

$$\begin{cases} \dot{x}(t) = \partial_\xi b(x(t), \xi(t)) \\ \dot{\xi}(t) = -\partial_x b(x(t), \xi(t)), \end{cases} \tag{2.2.13}$$

in the sense to be made precise below.

Proposition 2.2.4. *Let μ satisfy equation* (2.2.12) *with $b \in C_0^\infty(\mathbb{R}^{2d})$ real. Let be Φ the flow with trajectories given by* (2.2.13). *Then Φ is unique and, for any $a \in C_0^\infty(\mathbb{R}^{2d})$, one has*

$$\langle \mu_0, a \rangle_{\mathbb{R}^{2d}} = \langle \mu_t, a \circ \Phi_{-t} \rangle_{\mathbb{R}^{2d}}.$$

Proof. We only need to verify that $\frac{d}{dt}\big|_{t=\tau} \int a\circ\Phi_{-t}\, d\mu_t = 0$ for any τ. If $\tau = 0$, this comes straightforwardly from (2.2.12) and the vector field inducing the flow in (2.2.13). For $\tau \neq 0$, write $a\circ\Phi_{-t} = a\circ\Phi_{-\tau}\circ\Phi_{-t+\tau}$ and do the same calculations for the variable $\tilde{t} = t - \tau$ at 0 and the test function $\tilde{a} = a\circ\Phi_{-\tau}$. The unicity of Φ follows from an application of the Picard-Lindelöf theorem. □

Remark 2.2.5. Proposition 2.2.4 allows us to solve the differential system (2.2.12) with the pull-back $\mu_t = \Phi_t^* \mu_0$, where one has $\langle \Phi_t^* \gamma \, , a \rangle_{\mathbb{R}^{2d}} = \langle \gamma \, , a \circ \Phi_t \rangle_{\mathbb{R}^{2d}}$ for any measure γ on $\mathbb{R}^{2d}$, not being necessary to calculate Ψ_t^ε using equation (2.2.4). Numerically, this can save a tremendous amount of computation in studying the concentration of Ψ^ε over the time.

In order to have equations (2.2.11), (2.2.12) and Proposition 2.2.4 still valid for the Hamiltonian operator $\hat{H}^\varepsilon$, it is necessary to impose further conditions on the potential V so the standard symbolic calculus holds, as we have already said in Remark 2.2.2. If this is not the case, we can still try to re-derive "by hand" adapted formulæ for a correct symbolic calculus with the problematic potential (which indeed we will do progressively in Sections 4.4.1, 4.4.2 and 4.4.3 in Chapter 4).

Ideally, we would have basically to analyse the commutator $\frac{i}{\varepsilon}\left[\hat{H}^\varepsilon \, , \mathrm{op}_\varepsilon(a)\right]$ and show that it is approximatively in $L^2(\mathbb{R}^d)$ the pseudodifferential operator

$$\frac{i}{\varepsilon}\left[\hat{H}^\varepsilon \, , \mathrm{op}_\varepsilon(a)\right] = \mathrm{op}_\varepsilon\left(D(x, \xi, \partial_x, \partial_\xi)a\right) + \mathcal{O}(\varepsilon), \tag{2.2.14}$$

where $D(x, \xi, \partial_x, \partial_\xi)$ would be a partial differential operator or likewise to which we could seek an explicit form.

Having $V \in C^2(\mathbb{R}^d)$ allows us to obtain $D(x, \xi, \partial_x, \partial_x) = \xi \cdot \partial_x - \nabla V(x) \cdot \partial_\xi$, which gives the Liouville equation for the semiclassical measure:

$$\partial_t \mu(t, x, \xi) + \xi \cdot \partial_x \mu(t, x, \xi) - \nabla V(x) \cdot \partial_\xi \mu(t, x, \xi) = 0 \quad \text{in} \quad \mathcal{D}'(\mathbb{R} \times \mathbb{R}^{2d}), \tag{2.2.15}$$

or, in other words:

$$\begin{cases} \partial_t \mu_t(x, \xi) + \xi \cdot \partial_x \mu_t(x, \xi) - \nabla V(x) \cdot \partial_\xi \mu_t(x, \xi) = 0 \\ \mu_{t=0}(x, \xi) = \mu_0(x, \xi) \end{cases} \quad \text{in} \quad \mathcal{D}'(\mathbb{R}^{2d}). \tag{2.2.16}$$

Of course, for such a regular flow the Hamiltonian flow is well-posed, and Proposition 2.2.4 accomplishes the passage from Quantum to Classical Mechanics

2.2.3 Invariance phenomena

Let us now investigate how the invariance of a semiclassical measure through some flows may help localizing it, which will be particularly useful in Part III.

We will say that a flow Φ over $\mathbb{R}^{2d}$ is *dispersive* over $K \subset \mathbb{R}^{2d}$ if it is possible to find a sequence $(s_n)_{n \in \mathbb{N}_0}$ tending to ∞ with $s_0 = 0$ such that $\Phi_{s_n}(K) \cap \Phi_{s_m}(K) = \emptyset$ whenever $n \neq m$. Of course, the flow will be dispersive all over the region $\Phi_\Upsilon(K)$, with $\Upsilon = [0, \infty) \subset \mathbb{R}$.

Lemma 2.2.6. *Let μ be a finite and positive measure on $\mathbb{R}^{2d}$ that is invariant by the flow Φ on $K \subset \mathbb{R}^{2d}$,* i.e.*, such that $\mu(\Phi_t(K)) = \mu(K)$ for any $t \in \mathbb{R}$. Suppose also that Φ is dispersive over K. Then $\mu(K) = 0$.*

Proof. For any $N \in \mathbb{N}$, invariance by Φ yelds:

$$N\mu(K) = \mu\left(\bigcup_{n=1}^{N} \Phi_{s_n}(K)\right) \leqslant \mu(\mathbb{R}^{2d}) < \infty,$$

which cannot hold unless $\mu(K) = 0$. □

Proposition 2.2.7. *Let be $b \in C_0^\infty(\mathbb{R}^{2d})$ real and call Φ the phase space flow associated to it by system* (2.2.13)*. If a measure μ on $\mathbb{R}^{2d}$ satisfies*

$$\{b\,(x,\xi)\,, \mu(x,\xi)\} = 0, \tag{2.2.17}$$

then μ is invariant by Φ.

Proof. Show that, for any test function $a \in C_0^\infty(\mathbb{R}^{2d})$, $\frac{d}{dt}\big|_{t=0} \int a \circ \Phi_t \, d\mu = 0$ as in the proof of Proposition 2.2.4. □

Corollary 2.2.8. *In the same conditions of the proposition, suppose that μ is finite and positive, and that Φ is dispersive over some $K \subset \mathbb{R}^{2d}$. Then, for $\Upsilon = [0,\infty)$, one has $\mu\left(\Phi_\Upsilon(K)\right) = 0$.*

With these results in hand, let us suppose that the family $(\Psi^\varepsilon)_{\varepsilon>0}$ solves the equation

$$i\varepsilon^2 \partial_t \Psi_t^\varepsilon = \mathrm{op}_\varepsilon(b)\Psi_t^\varepsilon, \tag{2.2.18}$$

which can be interpreted as a version of (2.2.4) for times $t \sim \frac{t}{\varepsilon}$ asymptotically great. A dynamical equation for the Wigner measures of the family Ψ^ε can be obtained as in the previous section, by analysing the commutator in

$$\begin{aligned} \frac{d}{dt}\left\langle \mathrm{op}_\varepsilon\,(a)\,\Psi_t^\varepsilon\,, \Psi_t^\varepsilon\right\rangle &= \left\langle \frac{i}{\varepsilon^2}\left[\mathrm{op}_\varepsilon(b), \mathrm{op}_\varepsilon\,(a)\right]\Psi_t^\varepsilon\,, \Psi_t^\varepsilon\right\rangle \\ &= \frac{1}{\varepsilon}\mathrm{op}_\varepsilon\left(\{b\,,a\}\right) + \mathcal{O}(1), \end{aligned} \tag{2.2.19}$$

and then multiplying both sides of (2.2.10) by ε and taking the semiclassical limit as in (2.2.9):

$$\{b\,(x,\xi)\,, \mu(t,x,\xi)\} = 0 \qquad \text{in} \qquad \mathcal{D}'(\mathbb{R}\times\mathbb{R}^{2d}),$$

or equivalently, for every $t \in \mathbb{R}$:

$$\{b\,(x,\xi)\,, \mu_t(x,\xi)\} = 0 \qquad \text{in} \qquad \mathcal{D}'(\mathbb{R}^{2d}),$$

which means that the semiclassical measure of Ψ^ε does not charge the regions in the phase space where the flow is dispersive.

Remark 2.2.9. Observe that in this case continuity for $t \longmapsto \mu_t$ is not assured, as the derivative $\frac{d}{dt}\left\langle \mathrm{op}_\varepsilon\,(a)\,\Psi_t^\varepsilon\,, \Psi_t^\varepsilon\right\rangle$ is not necessarily bounded, contrarily to what happened in Remark 2.2.2.

Since μ gives the mass concentration of the solutions of (2.2.18), Proposition 2.2.7 and its corollary justify a classification of the (pseudo)-differential equations of type (2.2.18)[3] as dispersive or non-dispersive in certain regions of the phase space depending on the flow's character thereon.

Besides, μ can be used to study the mass concentration of the solutions of the standard equation (2.2.4) for long times at the scale $\frac{1}{\varepsilon}$, since it can be recovered from (2.2.18) after a change of variable of the sort. Ultimately, this says that if Ψ^ε are solutions to (2.2.4) with some b and μ satisfies (2.2.17) for some $\tilde{b}$, then for sufficient large times no mass is expected to be left in the regions where the flow associated to $\tilde{b}$ is dispersive, and this should be explicitly verified by a transport phenomenon along the flow generated by b, that should continuously take away all the mass initially spread over these regions.

[3] More precisely, for equations of type $i\varepsilon^\alpha \partial_t \Psi_t^\varepsilon = \mathrm{op}_{\varepsilon^\beta}(b)\Psi_t^\varepsilon$, with $\alpha > \beta > 0$ strictly.

2.3 Two-microlocal analysis

Now, let us define a new symbol class $S(p)$ composed by symbols $a \in C^\infty(\mathbb{R}^{2d+p})$ such that

- For each $\rho \in \mathbb{R}^p$, $(x,\xi) \longmapsto a(x,\xi,\rho)$ is compactly supported on $\mathbb{R}^{2d}_{x,\xi}$.
- There exists some $R_0 > 0$ and a function $a_\infty \in C^\infty(\mathbb{R}^{2d} \times \mathcal{S}^{p-1})$ such that, for $\|\rho\| > R_0$, one has $a(x,\xi,\rho) = a_\infty\left(x,\xi,\frac{\rho}{\|\rho\|}\right)$.

These symbols will be quantized as

$$\mathrm{op}^\sharp_\varepsilon(a(x,\xi,\rho)) = \mathrm{op}_\varepsilon\left(a\left(x,\xi,\frac{x'}{\varepsilon}\right)\right);$$

observe that the right-hand term above is just the banal quantization of a ε-dependent $\mathbb{R}^{2d}$ function as in (2.1.1).

Proposition 2.3.1. *There exists a measure ν_∞ on $\mathbb{R} \times \mathbb{R}^{2d-p} \times S^{p-1}$ and a trace class operator valued measure M on $\mathbb{R} \times \mathbb{R}^{2(d-p)}$, both positive, such that, for $a \in S(p)$ and $\Xi \in C_0^\infty(\mathbb{R})$,*

$$\begin{aligned}\mathrm{sc}\lim \int_{\mathbb{R}} \Xi(t)\left\langle \mathrm{op}^\sharp_\varepsilon(a)\Psi^\varepsilon_t\,,\,\Psi^\varepsilon_t\right\rangle dt \;&=\; \left\langle \mu(t,x,\xi)\mathbb{1}_{\{x'\neq 0\}}\,,\Xi(t)\,a_\infty\left(x,\xi,\frac{x'}{\|x'\|}\right)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}\\ &+\; \langle \delta(x')\otimes\nu_\infty(t,x'',\xi,\omega)\,,\Xi(t)\,a_\infty(x,\xi,\omega)\rangle_{\mathbb{R}\times\mathbb{R}^{2d}\times\mathcal{S}^{p+1}}\\ &+\; \mathrm{tr}\,\langle M(t,x'',\xi'')\,,\,\Xi(t)\,a^w(0,x'',\partial_y,\xi'',y)\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}}\,,\end{aligned} \tag{2.3.1}$$

where $a^w(0,x'',\partial_y,\xi'',y)$ is the Weyl quantization of the symbol $(y,\zeta) \longmapsto a(0,x'',\zeta,\xi'',y)$ with $\varepsilon = 1$ and μ is the usual Wigner measure related to Ψ^ε.

Furthermore, for a smooth compactly supported function $(x'',\xi'') \longmapsto T_{(x'',\xi'')}$ taking values on the set of compact operators on $\mathbb{R}^p$, one has

$$\langle M(t,x'',\xi'')\,,\,\Xi(t)\,T_{(x'',\xi'')}\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}} = \mathrm{sc}\lim \int_{\mathbb{R}\times\mathbb{R}^{2(d-p)}} \Xi(t)\,T_{(x'',\xi'')}U^\varepsilon_{(t,x'',\xi'')}dx''d\xi''dt,$$

where $U^\varepsilon_{(t,x'',\xi'')}$ is the trace class operator with kernel

$$kU^\varepsilon_{(t,x'',\xi'')}(y',x') = \int_{\mathbb{R}^{d-p}} \frac{e^{\frac{i}{\varepsilon}\xi''\cdot y''}}{(2\pi\varepsilon)^{d-p}}\,\Psi^\varepsilon_t\left(\varepsilon y',x''-\frac{y''}{2}\right)\overline{\Psi^\varepsilon_t\left(\varepsilon x',x''+\frac{y''}{2}\right)}dy''. \tag{2.3.2}$$

Finally, the terms in (2.3.1) are obtained respectively from those in the decomposition

$$a(x,\xi,\rho) = a(x,\xi,\rho)\left(1-\chi\left(\frac{x'}{\delta}\right)\right) + a(x,\xi,\rho)\left(1-\chi\left(\frac{\rho}{R}\right)\right)\chi\left(\frac{x'}{\delta}\right) + a(x,\xi,\rho)\chi\left(\frac{\rho}{R}\right)$$

in the limit when $\varepsilon \longrightarrow 0$, then $R \longrightarrow \infty$, and last $\delta \longrightarrow 0$, where χ is a cut-off function such that $0 \leqslant \chi \leqslant 1$, $\chi(x') = 1$ for $\|x'\| < \frac{1}{2}$ and $\chi(x') = 0$ for $\|x'\| \geqslant 1$.

Remark 2.3.2. If $p = d$, then $U^\varepsilon_t = \left|\tilde{\Psi}^\varepsilon_t\right\rangle\left\langle\tilde{\Psi}^\varepsilon_t\right|^*$ is just the adjoint of the projector over $\tilde{\Psi}^\varepsilon_t(x) = \varepsilon^{\frac{d}{2}}\Psi^\varepsilon(\varepsilon x)$, with kernel $kU^\varepsilon_t(x,y) = \tilde{\Psi}^\varepsilon_t(y)\overline{\tilde{\Psi}^\varepsilon_t(x)}$. It follows that

$$\mathrm{tr}\,(T\,U^\varepsilon_t) = \left\langle T\,\tilde{\Psi}^\varepsilon_t\,,\,\tilde{\Psi}^\varepsilon_t\right\rangle.$$

Then, because T is compact, in the limit $\varepsilon \longrightarrow 0$ one has that it is simply $\left\langle T\tilde{\Psi}_t, \tilde{\Psi}_t\right\rangle$, where Ψ_t is some weak limit of Ψ^ε_t.

A very general treatment of this result can be found in [43]. The introduction of U^ε is a trivial addition of ours in order to enlighten the calculations to come.

Remark 2.3.3. Observe that M induces a measure $\mathfrak{m}$ on $\mathbb{R}\times\mathbb{R}^{2d}$ by means of the formula

$$\begin{aligned}\left\langle\, \delta(x')\otimes\mathfrak{m}(t,x'',\xi,\rho)\,,\,\Xi(t)\,a(x,\xi,\rho)\,\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d+p}}\\ =\operatorname{tr}\left\langle\, M(t,x'',\xi'')\,,\,\Xi(t)\,a^w\left(0,x'',\partial_y,\xi'',y\right)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}}.\end{aligned}$$

Above, a has no need to be in $S(p)$; it is sufficient that it be compactly supported in all variables.

Lemma 2.3.4. *$M=0$ if and only if $\mathfrak{m}=0$.*

Proof. That $M=0$ implies $\mathfrak{m}=0$, it is obvious. For the converse, it is necessary to show that $\mathfrak{m}=0$ implies $\operatorname{tr}\langle M,T\rangle=0$ for all smooth compactly supported functions $(t,\,x'',\xi'')\longmapsto T_{(t,\,x'',\,\xi'')}$ taking values in the set of compact operators, since this is the set whose dual are the trace class operators.

Observe that it is sufficient to consider $T_{(t,\,x'',\,\xi'')}$ Hilbert-Schmidt, given that these operators are dense in the set of the compact ones. So, we can consider that it has a kernel $kT_{(t,x'',\,\xi'')}\in L^2\left(\mathbb{R}^{2p}_{x',y'}\right)$ and, defining

$$a(t,x,\xi,\rho)=\chi(x')\,\mathcal{F}_{y'\to\xi'}\left(kT_{(t,\,x'',\,\xi'')}\left(\rho+\frac{y'}{2},\rho-\frac{y'}{2}\right)\right)$$

with some $\chi\in C_0^\infty(\mathbb{R}^p)$, it follows that $T_{(t,\,x'',\,\xi'')}=a^w(t,0,x'',\partial_y,\xi'',y)$ and we are done. □

Lemma 2.3.5. *The measure $\mathfrak{m}$ is absolutely continuous with respect to $d\xi' d\rho$.*

Proof. Indeed, if $a(x,\xi,\rho)-b(x,\xi,\rho)=0$ unless for a set with null Lebesgue measure $d\xi' d\rho$, then $a^w(0,x'',\partial_y,\xi'',y)=b^w(0,x'',\partial_y,\xi'',y)$ and the result follows from the definition in Remark 2.3.3. □

Remark 2.3.6. In Example 11.1.3 in Chapter 11, we will prove that $\mathfrak{m}$ can actually be singular in all other variables, aside from the time, of course.

Lemma 2.3.7. *The semiclassical measure μ decomposes as*

$$\begin{aligned}\mu(t,x,\xi)=\mu(t,x,\xi)\mathbb{1}_{\{x'\neq0\}}+\delta(x')\otimes\int_{\mathcal{S}^{p-1}}\nu_\infty(t,x'',\xi,d\omega)\\ +\,\delta(x')\otimes\left(\int_{\mathbb{R}^p}\mathfrak{m}_{(\xi',\rho)}(t,x'',\xi'')\,d\rho\right)d\xi',\end{aligned}\tag{2.3.3}$$

where ν_∞ is as in Proposition 2.3.1 and $\mathfrak{m}_{(\xi',\rho)}(t,x'',\xi'')\,d\rho\,d\xi'=\mathfrak{m}(t,x'',\xi,\rho)$.

Proof. If $a\in C_0^\infty$, define $\tilde a(x,\xi,\rho)=a(x,\xi)$ for all $\rho\in\mathbb{R}^p$. Thus, $\tilde a\in S(p)$ and $\operatorname{op}_\varepsilon(a)=\operatorname{op}^\sharp_\varepsilon(\tilde a)$, and we can use Proposition 2.3.1. □

More generally, this kind of two-scale analysis can be used to analyse the concentration of the Wigner measures over any submanifold Λ of the phase space such that the restriction of the symplectic form $\sigma=dx\wedge d\xi$ on $T^*\Lambda$ is of constant rank[41]. In this thesis, we only need to specialise it to spaces of the form $x'=0$ in Part II and $\xi'=0$ in Part III, whose due modifications will be presented in Section 9.4 along with a comprehensive treatment of the geometric properties of ν_∞ and M.

Part II

Conical Singularities

Chapter 3

Presenting the problem – potentials with conical singularities

Part II of this thesis was published independently in [30].

3.1 Statement of the problem

Classically, a particle with mass $m = 1$ submitted to a time- and momentum-independent smooth potential V in $\mathbb{R}^d$ is constrained to move following the phase space trajectory given by the Hamilton equations

$$\left\{ \begin{array}{l} \dot{x}\left(t\right) = \xi\left(t\right) \\ \dot{\xi}\left(t\right) = -\nabla V\left(x\left(t\right)\right). \end{array} \right. \tag{3.1.1}$$

Smoothness in V guarantees that the equations above have a unique solution $(x(t), \xi(t))$ around all initial condition (x_0, ξ_0) (*i.e.*, for t sufficiently small), thus we can define the classical Hamiltonian flow Φ by setting $\Phi_t\left(x_0, \xi_0\right) = (x(t), \xi(t))$. Further conditions on the regularity and growth rate of V imply more good properties, so if $\nabla^2 V$ is bounded, one can extend $\Phi_t(x_0, \xi_0)$ for all $t \in \mathbb{R}$, for any (x_0, ξ_0) in the phase space[97].

In Quantum Mechanics, the state evolution of a similar system is described by a function $\Psi^\varepsilon \in L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^d)\right)$ obeying to the Schrödinger equation with initial data

$$\left\{ \begin{array}{l} i\varepsilon\partial_t\Psi^\varepsilon_t\left(x\right) = -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon_t(x) + V(x)\Psi^\varepsilon_t(x) \\ \Psi^\varepsilon_{t=0}\left(x\right) = \Psi^\varepsilon_0\left(x\right), \end{array} \right. \tag{3.1.2}$$

where the initial $L^2(\mathbb{R}^d)$ data satisfy $\|\Psi^\varepsilon_0\|_{L^2(\mathbb{R}^d)} = 1$ and $\varepsilon \ll 1$ is a parameter generally reminiscent from some rescaling procedure, but that can also be seen as the Planck's constant in a system with mass of order $m \approx 1$, in which case the Wigner measures can be viewed as the classical limits of the system's mass distribution, as we will explain next.

If V satisfies the Kato-Rellich conditions (V continuous and $V(x) \lesssim \|x\|^2$), then the Hamiltonian operator

$$\hat{H}^\varepsilon = -\frac{\varepsilon^2}{2}\Delta + V \tag{3.1.3}$$

with domain in the Sobolev space $H^2(\mathbb{R}^d)$ is essentially self-adjoint ([67],[97]) and (3.1.2) has a unique solution for all $t \in \mathbb{R}$, which is given by

$$\Psi^\varepsilon_t = e^{-\frac{i}{\varepsilon}t\hat{H}^\varepsilon}\Psi^\varepsilon_0.$$

It happens that a very large class of relevant problems do not present potentials with all such regularity. For instance: *conical potentials*, which are of the form

$$V(x) = V_S(x) + \|g(x)\|\, F(x), \tag{3.1.4}$$

where we make the following technical assumptions:

- V and V_S satisfy each one the Rellich conditions.
- F and V_S are $C^\infty(\mathbb{R}^d)$ and there is some non-decreasing positive K-sub-additive[1] polynomial $\mathfrak{p}$ that bounds them and also ∇F.
- $g : \mathbb{R}^d \longrightarrow \mathbb{R}^p$ with $1 \leqslant p \leqslant d$, ∇g is full rank and $\Lambda = \{g(x) = 0\} \neq \emptyset$.

As we shall see, these potentials raise interesting mathematical questions.

Similar problems have been treated in works like [8], [17] and [18] in a probabilistic way. In other works authors have been analysing the deterministic behaviour of the Wigner measures under the conical potentials defined above, more noticeably in [45], where they found a non-homogeneous version of (2.2.15) whose inhomogeneity is an unknown measure supported on

$$\Omega = \left\{(x, \xi) \in \mathbb{R}^{2d} \,:\, g(x) = 0 \text{ and } \nabla g(x)\, \xi = 0\right\},$$

a set onto which it is not generally possible to extend the classical flow in a unique manner, although it is possible everywhere else.

Remark 3.1.1. The set Ω corresponds exactly to the tangent bundle to Λ, since any curve γ over Λ (*i.e.*, such that $g(\gamma(t)) = 0$) passing on x at $t = 0$ must satisfy $\nabla g(x)\dot{\gamma}(0) = 0$. In our work, however, we stay within a structure of phase space, so it will be natural to identify Ω as the cotangent bundle $T^*\Lambda$.

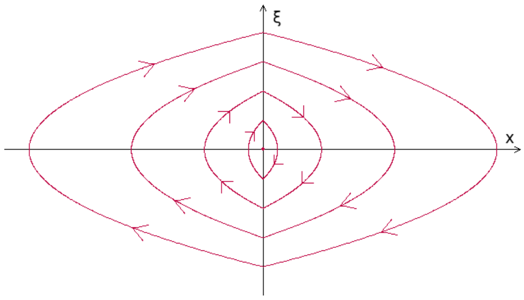
This suggests an intriguing possibility involving irregular potentials: what happens to the Wigner measures in a system where the potential allows a complete quantum treatment, but causes the classical flow to be ill-defined? Is there some selection principle from the quantum-classical correspondence that could provide information enough for describing the transport of the measure where the classical flow fails?

To fix some ideas, forget for a moment about the measures and think of a classical particle submitted to conical potentials like $V(x) = \pm |x|$. Naturally, the trajectories are well-defined everywhere away from the line $x = 0$, and it turns out that they can be continuously extended onto $x = 0$ in a unique manner provided that $\xi \neq 0$, as in Figure 3.1.1.

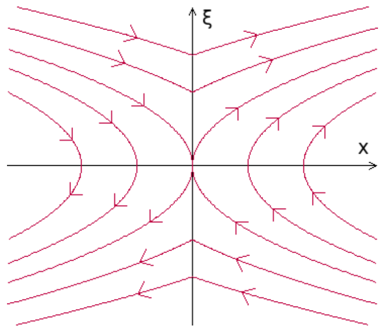
In the case $V(x) = +|x|$, the flow can be uniquely defined even over $\xi = 0$ by setting it constant at the origin, as shown in Figure 3.1.1(a); more generally, in higher dimensional cases, like for $x \in \mathbb{R}^d$, $x = (x', x'')$ with $x' \in \mathbb{R}^p$ and $V(x) = \|x'\|$, there is still room for the particle to move inside the singular set $\Omega = \{x' = 0 \text{ and } \xi' = 0\}$ and it must have some non-ambiguous behaviour therein, induced by the unique quantum evolution of Ψ_t^ε and their well-defined concentration to μ_t. However, the dynamics in Ω is classically unknown, for ∇V makes no sense for $x' = 0$, so we cannot rely on the sole Hamiltonian trajectories to characterize the transport phenomenon that the semiclassical measure undergoes over the singularities.

Furthermore, there are other kinds of difficulties. In the case $V(x) = -|x|$, even in dimension 1 there is no unique extension for the flow all over the phase space. As we can

[1]This is: there is $K \geqslant 1$ such that $\mathfrak{p}(x + y) \leqslant K\,(\mathfrak{p}(x) + \mathfrak{p}(y))$.



(a) $V(x) = |x|$. At the origin the trajectory is constant.



(b) $V(x) = -|x|$. At the origin the flow is not well-defined.

Figure 3.1.1: A glance on the classical flows for the potentials $V(x) = \pm|x|$ near the origin. The arrows indicate their orientation.

see in Figure 3.1.1(b), when coming from the right-hand side below, there are different alternative trajectories after reaching $x = 0$ with zero momentum: going back to the right upwards, crossing to the left downwards, staying at $(0\,,0)$, or staying there for a moment and then resume moving to one or to the other side.

Let us treat this problem in three different steps.

3.2 First question: the dynamics

In [45], the authors proved that the Hamiltonian flow can always be continuously extended in a unique manner to $\Lambda \setminus \Omega$ and that, whenever the Wigner measure does not charge the singularities in the phase space, *i.e.*, while $\mu_t(\Omega) = 0$, then μ follows these unique continuous extensions. This result is grounded on the facts that μ_t does not charge the set $\Lambda \setminus \Omega$ for more than a negligible time, more precisely that $\mu_t(\Lambda \setminus \Omega) = 0$ almost everywhere in $\mathbb{R}$ with respect to dt (for a matter of completeness, we re-obtain this result in Lemma 4.5.1), and that the measures obey to the standard Liouville equation with V away from Λ, where the potential is regular.

We will obtain in Chapter 4 a complete description of the dynamics to which the semiclassical measures ought to obey, including near and inside the singularities, by driving an approach similar to that of [45], which makes an extensive use of *symbolic calculus* (Section 2.1) and *two-microlocal measures* (Section 2.3):

Theorem 3.2.1. *Let Ψ^ε be the solution to the system* (3.1.2) *with a conical potential of the form* (3.1.4)*, and denote $\Lambda = \left\{x \in \mathbb{R}^d : g(x) = 0\right\}$. Then the correspondent Wigner measures μ obey to the $\mathcal{D}'(\mathbb{R} \times \mathbb{R}^{2d})$ equation:*

$$\begin{aligned}(3.2.1)\qquad &\left(\partial_t + \pi_{T_x^*\Lambda}\xi \cdot \partial_x - \pi_{T_x^*\Lambda} \nabla V_S|_\Lambda(x) \cdot \partial_\xi\right) \mathbb{1}_{T^*\Lambda}\, \mu(t,x,\xi) \\ &\qquad + \left(\partial_t + \xi \cdot \partial_x - \nabla V(x) \cdot \partial_\xi\right) \mathbb{1}_{(T^*\Lambda)^c}\, \mu(t,x,\xi) = 0,\end{aligned}$$

where $\mathbb{1}_{T^*\Lambda}$ is the indicatrix of $T^*\Lambda = \Omega$ (and $\mathbb{1}_{(T^*\Lambda)^c}$ of its complement inside $\mathbb{R}^{2d}$) and for each $x \in \Lambda$, $\pi_{T_x^*\Lambda}$ is the orthogonal projector over $T_x^*\Lambda = \ker \nabla g(x)$ inside $\mathbb{R}^d$.

Furthermore, decomposing $\mathbb{R}^{2d}$ in a neighbourhood of Λ as the bundle $E\Lambda$ with fibres $E_\sigma\Lambda = T_\sigma^*\Lambda \oplus N_\sigma^*\Lambda \oplus N_\sigma\Lambda$ (and elements (σ,ζ,η,ρ)), there exists a measure ν over

$\mathbb{R} \times ES\Lambda$, where $ES_\sigma\Lambda = T^*_\sigma\Lambda \oplus {}^{N_\sigma\Lambda}\!\diagup_{\mathbb{R}^+_*}$, satisfying the asymmetry condition

$$\int_{N_\sigma\Lambda/\mathbb{R}^+_*} \left(\nabla_\rho V_S(\sigma) + F(\sigma)^t \nabla g(\sigma)\,\omega\right) \nu\left(t,\sigma,\zeta,d\omega\right) = 0 \quad \text{in } \mathcal{D}'\left(\mathbb{R}\times T^*\Lambda\right) \tag{3.2.2}$$

and such that

$$\mathbb{1}_{T^*\Lambda}\,\mu\left(\sigma,\zeta,\eta,\rho\right) \;=\; \delta(\rho)\otimes\delta(\eta)\otimes\int_{N_\sigma\Lambda/\mathbb{R}^+_*} \nu\left(t,\sigma,\zeta,d\omega\right).$$

Remark 3.2.2. Observe that equation (3.2.1) is the sum of two Liouville terms, one for the potential V outside Ω and another for $V_S|_\Lambda$ over it. Usual transport under V is assured away from Ω by [45], thus, if no trajectories outside Ω lead to or from it, these both terms are shown to cancel on their own[2] and the equation decouples into two independent transport phenomena, one inside and the other outside Ω, the regularity of the insider flow being guaranteed by the Picard-Lindelöf theorem, as $V_S|_\Omega$ is smooth in the topological space Ω.

Remark 3.2.3. The second part of the theorem, the asymmetry formula, will be discussed ahead in Section 3.3 and turns out to indicate that any mass that stays on the singularity will be in static equilibrium over it.

Remark 3.2.2 immediately gives:

Theorem 3.2.4. *In the same conditions of Theorem 3.2.1, suppose that no Hamiltonian trajectories lead into Ω. Call Φ the Hamiltonian flow defined by the trajectories induced by V for $(x,\xi)\notin\Omega$ and by $V_S|_\Lambda$ for $(x,\xi)\in\Omega$. Then, writing $\mu(t,x,\xi) = \mu_t(x,\xi)dt$, one has $\mu_t = \Phi^*_t\mu_0$ for all $t\in\mathbb{R}$, where μ_0 is the Wigner measure of the family $(\Psi^\varepsilon_0)_{\varepsilon>0}$.*

More precisely, suppose that the Hamiltonian flow Φ can be extended in a unique way everywhere in a region $\Gamma\subset\mathbb{R}^{2d}$. It is sufficient in Theorem 3.2.4 that we choose a time interval $I\subset\mathbb{R}$ such that $\Phi_I\left(\operatorname{supp}(\mu_0)\right)\subset\Gamma$ to assure the transport for any $t\in I$; this recovers the result in [45] for a particular choice where $\Gamma\cap\Omega=\emptyset$. In words, it is sufficient that our measure transported by the flow does not hit any point where the trajectories split, the fact that it may charge the singularities being irrelevant.

3.3 Second question: the regime change

Now, what happens if some trajectories hit Ω? First, realize that in this case there is never uniqueness, since there are necessarily the outgoing trajectory (which is the reverse of the incoming one) and the one whose projection on $T^*\Lambda$ evolves freely and, more importantly, whose projection on $N^*\Lambda$ remains static, what is always kinetically admissible (with $\nabla g(x)\xi = 0$, the velocity normal to Λ is 0, for $\ker\nabla g(x)$ is actually $T^*_x\Lambda$, as informs Theorem 3.2.1). The equation in Theorem 3.2.1 says that either a transfer of mass between these two regimes, the insider and the outsider, and the continuation of the exterior transport are possible to happen, but gives no more information.

The second part of the theorem, however, may solve the question. It has got a rich geometric interpretation, saying that the mass distribution on Ω has some asymmetry around

[2]To see this, just test μ against functions in $C^\infty_0\left(\mathbb{R}^{2d}\setminus\Omega\right)$ and consider the local conservation of mass.

Λ due to the "shape" $F^t\nabla g$ of the conical singularity, and that it is deformed by an exterior normal force $-\partial_\rho V_S$, in such a manner that the portion of mass that remains over the singularity will be in static equilibrium.

Indeed, the measure ν gives the mass distribution in a sphere bundle with fibres $S_\sigma\Lambda = N_\sigma\Lambda/_{\mathbb{R}_+^*}$ around the singularity, *i.e.*, the directions ω in the exterior space from where the solutions Ψ^ε concentrate more or less intensively to the singular points.

If $\nu = 0$, then of course the measure does not stay at the singularity, so it necessarily continues under the exterior regime (regardless of whether it is unambiguously defined or not) and we got all the information ν may give; let us then suppose $\nu \neq 0$.

Loosely, let us also consider ν as a function of (σ, ζ) (as if it was absolutely continuous with respect to $d\sigma d\zeta$) and let us say that $\int_{S_\sigma\Lambda} \nu(t, \sigma, \zeta, d\omega)$ gives the total mass $\mathcal{M}$ on the point (σ, ζ) (though it actually gives a mass density over the phase space) at the instant t, supposed not to be 0. Naturally, $\int_{S_\sigma\Lambda} \omega\, \nu(t, \sigma, \zeta, d\omega)$ gives the average vector of concentration to this point, whose normalization by $\mathcal{M}$ we will call $\vec{D}(\sigma)$.

Remark 3.3.1. Realize that the speed the mass may have tangentially to the singular space Λ, that we call ζ, plays no role in dictating how the quantum concentration will happen thereon; with simple hypotheses on the family $(\Psi_0^\varepsilon)_{\varepsilon>0}$ (like ε-oscillation, see [55]), one has $\int \mu(x, d\xi) < \infty$, and the same for ν since $\nu \ll \mu$, so we could be working directly with $\int_{ES_\sigma\Lambda} \nu(t, \sigma, d\zeta, d\omega)$.

Well, the derivative of a potential is a force, so let us call $\vec{F}^\perp(\sigma) = -\partial_\rho V_S(\sigma)$ the force normal to the singular manifold Λ at the point σ. Consequently, the asymmetry formula in Theorem 3.2.1 is imposing a simple condition on the mass concentration:

$$F(\sigma)^t \nabla g(\sigma) \vec{D}(\sigma) = \vec{F}^\perp(\sigma), \tag{3.3.1}$$

which is to say that, in average, the mass should concentrate alongside the exterior normal force $\vec{F}^\perp$. How strong the concentration will be there with respect to the other points, or whether it is going to be attractive or repulsive, will depend on the shape of the conical singularity at the different points of Λ, described (so as to say) by $F^t\nabla g$.

An example is illustrated in Figure 3.3.1 below.

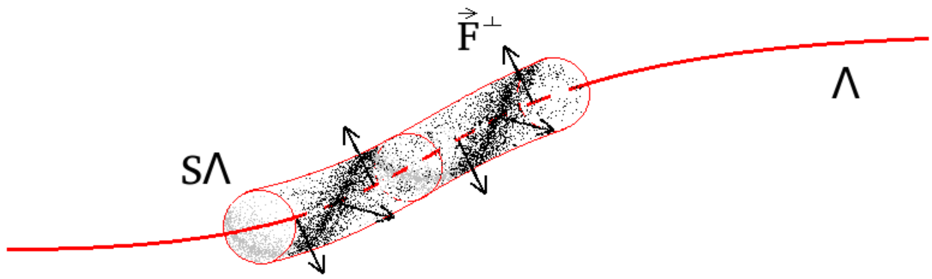


Figure 3.3.1: Above, we depict Λ encircled by its normal bundle in sphere $S\Lambda$ (with fibres $S_\sigma\Lambda = N_\sigma\Lambda/_{\mathbb{R}_+^*}$). The mass concentration given by ν is represented by the more or less strongly shadowed regions, and is directed by the normal force $\vec{F}^\perp$ which is spinning around Λ in the example. Here, we took $F(\sigma) = 1$ and $\nabla g(\sigma) = \mathbb{1}$.

The reason why we have said that equation (3.2.2) is a condition of equilibrium is that the expression inside the integral is similar to what would be the total force normal to Λ, *i.e.* $-\partial_\rho V$, when calculated on Λ (where $g = 0$) and making sense of ω as some limit of

$\frac{1}{\|\nabla g(\sigma)^{-1}g(x)\|}\nabla g(\sigma)^{-1}g(x)$ (a vector in $N_\sigma\Lambda$) when x approaches the singularity from a particular direction. So we are also tempted to interpret (3.2.2) as saying that the total force normal to Λ on some mass staying on the singularity, to be given by the integral, is 0: this mass is in static equilibrium.

Besides, in formula (3.3.1), we have $\left\|\vec{D}(\sigma)\right\| \leqslant 1$, since $\vec{D}(\sigma)$ is an average of norm 1 vectors in $N_\sigma\Lambda$. Consequently, we must have $\left\|F(\sigma)^t\nabla g(\sigma)\right\| \geqslant \left\|\vec{F}^\perp(\sigma)\right\|$ not to be led to an absurd. If this is not the case, then we must have $\nu = 0$ in order to satisfy the asymmetry condition trivially, which means that the Wigner measure will not stay on the singularity. This reasoning will be made rigorous in Section 5.1, where we will prove:

Theorem 3.3.2. *If for some $\sigma \in \Lambda$ one has $\left\|F(\sigma)^t\nabla g(\sigma)\right\|_{\mathcal{L}(N_\sigma\Lambda)} < \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}$, then there exists a neighbourhood $\Gamma \subset \Lambda$ of σ such that $\nu = 0$ over $\mathbb{R} \times ES\Gamma$, where $ES_\sigma\Gamma = T^*_\sigma\Gamma \oplus {}^{N_\sigma\Gamma}\!/_{\mathbb{R}^+_*}$.*

Once established that in some cases the mass is forbidden to stay over the singularity, it is worth studying more deeply the ways it can get in and out Ω:

Theorem 3.3.3. *Supposing $\left\|F(\sigma)^t\nabla g(\sigma)\right\|_{\mathcal{L}(N_\sigma\Lambda)} < \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}$, for any trajectory $(x(t), \xi(t))$ leading out from or into Ω in $\sigma \in \Lambda$ at $t_0 \in \mathbb{R}$, set the $N_\sigma\Lambda$ vector $\rho(t) = \frac{2}{(t-t_0)^2}\nabla g(\sigma)^{-1}g(x(t))$; then, if $\lim_{t\to t_0^\pm}\frac{\rho(t)}{\|\rho(t)\|}$ is well-defined, $\rho(t)$ also has well-defined lateral limits $\rho_0^\pm$ when $t \longrightarrow t_0^\pm$, which are non-zero roots of*

$$\rho_0 = -\partial_\rho V_S(\sigma) - F(\sigma)^t\nabla g(\sigma)\frac{\nabla g(\sigma)\rho_0}{\|\nabla g(\sigma)\rho_0\|}. \tag{3.3.2}$$

Conversely, for any ρ_0^+ and ρ_0^- satisfying (3.3.2)*, there exists a unique continuous extension of the classical flow which passes by σ at t_0 without staying on σ and whose correspondent limits $\lim_{t\longrightarrow t_0^\pm}\rho(t)$ exist and are equal to $\rho_0^\pm$.*

If (3.3.2) *has no non-zero roots, then no trajectory leads in or out Ω in σ.*

If $\|F(\sigma)^t\nabla g(\sigma)\|_{\mathcal{L}(N_\sigma\Lambda)} \geqslant \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}$, then $\rho(t)$ may converge laterally to 0 even if $\frac{1}{\|\nabla g(\sigma)\rho(t)\|}\nabla g(\sigma)\rho(t)$ has a well-defined lateral limit that we denote $\frac{1}{\|\nabla g(\sigma)\rho_0\|}\nabla g(\sigma)\rho_0$. We will abusively call ρ_0 "zero roots" of (3.3.2) and say that trajectories reach or leave Ω in σ following the respective directions $\rho_0^\pm$ if $\lim_{t\to t_0^\pm}\frac{1}{\|\nabla g(\sigma)\rho(t)\|}\nabla g(\sigma)\rho(t)$ exists and is equal to $\frac{1}{\|\nabla g(\sigma)\rho_0^\pm\|}\nabla g(\sigma)\rho_0^\pm$. Sometimes it may be that an incoming trajectory only approaches this limit asymptotically at $t_0^- = \infty$.

Theorem 3.3.4. *If $\|F(\sigma)^t\nabla g(\sigma)\|_{\mathcal{L}(N_\sigma\Lambda)} \geqslant \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}$, at least one of the following affirmations holds:*

- *Equation* (3.3.2) *has non-zero roots $\rho_0^\pm$ and there are unique trajectories leaving and arriving on Ω in σ through the directions $\rho_0^\pm$;*
- *Equation* (3.3.2) *has "zero roots", in the sense that there are $\rho_0 \neq 0$ such that*

$$F(\sigma)^t\nabla g(\sigma)\frac{\nabla g(\sigma)\rho_0}{\|\nabla g(\sigma)\rho_0\|} + \partial_\rho V_S(\sigma) = 0, \tag{3.3.3}$$

and either there is no trajectories reaching Ω in σ through ρ_0, or they exist but do not arrive onto Ω within any finite time;

- *The classical flow does not touch Ω in σ through any well-defined direction.*

Remark 3.3.5. In any case, if equation (3.3.2) has no roots ("zero" or non-zero), then no classical trajectory passes by Ω in $\sigma \in \Lambda$.

Remark 3.3.6. In [31], we will endeavour a more precise study of the link between ν and the classical flow, generalizing the link between Theorem 3.3.2 and Theorems 3.3.3 and 3.3.4.

In Section 5.1 we will work out the proof of Theorems 3.3.2, 3.3.3 and 3.3.4 in coordinates that are more suitable to understand $\rho(t)$ as an approaching direction. Besides, we will see in Section 5.3, by means of a number of examples, that these results allow a full classification of the types of trajectories that may reach or stay on the singularities. In some cases, like for $d = 1$ or $V(x) = \pm\|x\|$ in $\mathbb{R}^d$, they allow a full resolution of the problem when the inequality in Theorem 3.3.2 holds, since by solving explicitly (3.3.2) one can verify that there is only a unique trajectory leading in and out the singularity without staying thereon, and necessarily the measures will follow it and not charge Ω.

In short, so far we have seen that whenever we have a well-defined flow, we know what the semiclassical measures do: they are transported thereby. If the flow presents trajectory splits, they necessarily happen on Ω, where there is always the possibility of regime change between outsider and insider flows. Then, thanks to the measure ν, we may be able to obtain enough information to decide whether the measures stay or not on the singularity, and in case they stay, we know that they will be carried by the flow generated by $V_S|_\Lambda$.

3.4 Third question: trajectory crossings

Finally, a last problem is: if a measure does not stay on Ω and continues in the exterior flow, but even though there are different trajectories to take, can we derive from the well-posed quantum evolution some general criterion for choosing the actual trajectories that the measure will follow? Is there any selection principle for the classical movement of a particle under such conical potentials?

As we will see in Section 6.2, the answer is negative. The path a Wigner measure (or a particle) takes after its trajectory splits depends crucially on its quantum state concentration, so any selection principle making appeal only to purely classical or semiclassical information is to be dismissed.

This can be justified by:

Theorem 3.4.1. *Let be $V(x) = -|x|$ in $\mathbb{R}$ and μ^1 and μ^2 the Wigner measures associated to the solutions of* (3.1.2) *with initial data*

$$\Psi_0^{\varepsilon,1}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}}\Psi^1\left(\frac{x}{\sqrt{\varepsilon}}\right) \quad \text{and} \quad \Psi_0^{\varepsilon,2}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}}\Psi^2\left(\frac{x}{\sqrt{\varepsilon}}\right)e^{-i\varepsilon^{\beta-1}x},$$

with $0 < \beta < \frac{1}{10}$, $\Psi^1, \Psi^2 \in C_0^\infty(\mathbb{R})$ and Ψ^1 supported on $x > 0$. Then, for $t \leqslant 0$,

$$\mu_t^1(x,\xi) = \mu_t^2(x,\xi) = \delta\left(x - \frac{t^2}{2}\right) \otimes \delta\left(\xi + t\right);$$

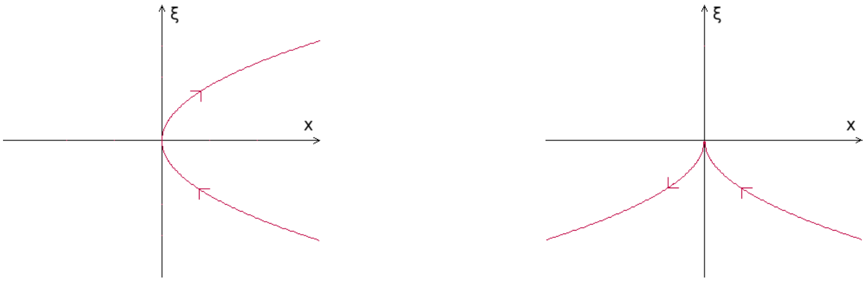
nevertheless, for $t > 0$,

$$\mu_t^1(x,\xi) = \delta\left(x - \frac{t^2}{2}\right) \otimes \delta\left(\xi - t\right)$$

whereas

$$\mu_t^2(x,\xi) = \delta\left(x + \frac{t^2}{2}\right) \otimes \delta(\xi + t)\,.$$

In pictures, the particle μ^1 follows the path in Figure 3.4.1(a), and the particle μ^2 moves as in Figure 3.4.1(b).



(a) Trajectory of μ^1. (b) Trajectory of μ^2.

Figure 3.4.1: Trajectories followed by two different particles, coinciding for $t \leqslant 0$, but then diverging for $t > 0$, which dismisses any selection principle based only on classical information about the problem.

This result will be obtained with the help of approximative solutions of (3.1.2) called *wave packets*, which are $L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^d)\right)$ functions generally of the form

$$\varphi_t^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} v_t\left(\frac{x - x(t)}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}[\xi(t)\cdot(x-x(t))+S(t)]}$$

(S is the classical action), to be properly introduced in Section 6.1. The standard methods using wave packet presented in that section, however, only apply for smooth flows, and in both cases the trajectories in Figure 3.4.1 have problems over the axis $x = 0$, not to speak about the lack of regularity of V.

In the case of the returning particle, the problem will be solved by decomposing the initial data into two pieces, for $x > 0$ and $x < 0$, and treating each one with a standard wave packet set to follow a different parabola. We will see in Proposition 6.2.1 that the Wigner measure initially set on the singularity will break out into two pieces μ^+ and μ^- with weights given by the total mass of the initial data over $x > 0$ and $x < 0$ respectively, $\int_0^\infty |v_0(x)|^2 dx$ and $\int_{-\infty}^0 |v_0(x)|^2 dx$, each piece gliding to a different side as in Figure 3.4.2.

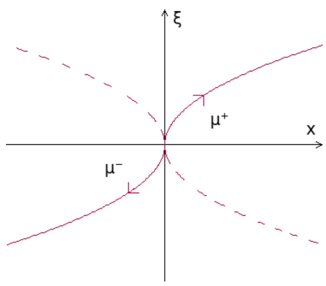


Figure 3.4.2: Trajectories followed by the measures μ^+ (right) and μ^- (left). The full line indicates the path for $t \geqslant 0$, whereas the dashed line indicates the past trajectories that the measures ought to have followed in $t < 0$ to reach the singularity.

Yet, this does not give a full example of non-unicity as in Theorem 3.4.1, since, if we evolve the pieces μ^+ and μ^- to the past, we realize that they do not come from the same side, and this fact could indicate some kind of selection principle.

Constructing a quantum solution whose semiclassical measure behaves like in Figure 3.4.1(b) will be more difficult and will require us to consider a family of wave packets following different trajectories with smaller and smaller initial momenta η, that in some sense converge to the aimed path with $\eta = 0$, as illustrated in Figure 3.4.3. We will then study the concentration of the wave packets with ε going to 0 at the same time as the trajectories concentrate, by making η go to 0 with a suitable power of ε.

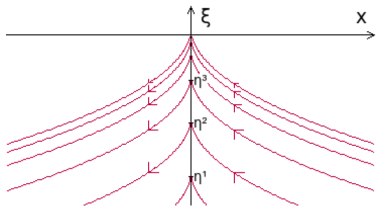


Figure 3.4.3: The trajectories (6.2.10) for $|\eta| = |\eta^1| > |\eta^2| > |\eta^3|$..., approaching the aimed one with $\eta = 0$.

Chapter 4

The dynamics

In view of the developments in Section 2.1, from equation (2.2.10) we are left with the analysis of the commutator

$$\frac{i}{\varepsilon}\left[\hat{H}^{\varepsilon}\,, \mathrm{op}_{\varepsilon}\,(a)\right] = \frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}\Delta\,, \mathrm{op}_{\varepsilon}\,(a)\right] + \frac{i}{\varepsilon}\left[V_S\,, \mathrm{op}_{\varepsilon}\,(a)\right] + \frac{i}{\varepsilon}\left[\|g(x)\|F(x)\,, \mathrm{op}_{\varepsilon}\,(a)\right].$$

We will look separately into each of these terms. The first one is kinetic, the other two dynamical. The first and the second are regular enough so one can use standard symbolic calculus; this presents no difficulties and we will treat them explicitly in Sections 4.2 and 4.3 only for a matter of completeness.

The third term is complicate because of the conical singularities it presents, which will require us to employ the two-microlocal analysis in Section 2.3. This strategy was followed in [45], but here we will describe the two-microlocal measures in more details. Prior to proceeding to this kind of analysis, however, we will need to restrict ourselves to the case where $g(x) = x'$, with $x = (x', x'')$, $x' \in \mathbb{R}^p$ and $1 \leqslant p \leqslant d$, in other words, to the case where the manifold Λ formed by the singularities is actually a subspace $\mathbb{R}^p$.

It is in this context that we will be able to prove Proposition 4.5.6, which is a particular version of Theorem 3.2.1 for $\Lambda = \mathbb{R}^p$. Reducing the general case to this one is the subject of next section.

4.1 Reducing Λ to a subspace $\mathbb{R}^{d-p}$

For a general conical potential, thanks to $\nabla g(x)$ having maximal rank we can define a local change of coordinates ϕ in neighbourhoods of $\mathbb{R}^d$ where

$$\begin{aligned} z &= \phi\,(x) \\ \begin{pmatrix} z' \\ z'' \end{pmatrix} &= \begin{pmatrix} g(x) \\ f(x) \end{pmatrix} \end{aligned}$$

for some function $f : \mathbb{R}^d \longrightarrow \mathbb{R}^{d-p}$ locally depending on g in such a manner that $\nabla f(x)$ has maximal rank and, if $x \in \Lambda$, then $\ker \nabla f(x)$ is orthogonal to $\ker \nabla g(x)$[1].

[1]Such f may be constructed as follows: let be $\mathcal{A}$ an open neighbourhood of Λ; choose $\kappa : \mathcal{A} \longrightarrow \mathbb{R}^{d-p}$ a local diffeomorphism; take $\tilde{U} \subset \mathbb{R}^d$ a cylindrical neighbourhood of Λ such that $\tilde{U} \cap \Lambda \subset \mathcal{A}$. Pick up an open $U \subset \tilde{U}$, so $x \in U$ is given in geodesic coordinates by $x = (\tilde{\sigma}, \eta)$ for some $\sigma \in \mathcal{A}$ with coordinates $\tilde{\sigma}$ and $\eta \in N_\sigma\Lambda$. Define $f : U \longrightarrow \mathbb{R}^{d-p}$ as $f(x) = \kappa(\sigma)$. It follows that $\nabla f(x)$ is diffeomorphic over $T_\sigma\Lambda$ and null over $N_\sigma\Lambda$, but since $T_\sigma\Lambda = \ker \nabla g((\tilde{\sigma}, 0))$ (see Remark 3.1.1), $\ker \nabla f((\tilde{\sigma}, 0)) \perp \ker \nabla g((\tilde{\sigma}, 0))$ and we are done.

Now, for the sake of clarity let us consider the coordinate change in tangent space induced by ϕ:

$$\begin{array}{rcl} \tilde{\zeta} & = & \nabla\phi\,(x)\,\xi \\ \left(\begin{array}{c} \tilde{\zeta}' \\ \tilde{\zeta}'' \end{array}\right) & = & \left[\begin{array}{c} \nabla g(x) \\ \nabla f(x) \end{array}\right]\xi. \end{array}$$

Writing $\mathbb{R}^d = \ker\nabla g(x) \oplus \ker\nabla f(x)$, we have the decomposition

$$\xi = \pi_g(x)\,\xi + \pi_f(x)\,\xi,$$

where $\pi_g(x)$ and $\pi_f(x)$ are suitable projectors inside $\mathbb{R}^d$ over the kernels of $\nabla g(x)$ and $\nabla f(x)$; if $x \in \Lambda$, they are orthogonal. Realize that $\nabla f(x)|_{\ker\nabla g(x)}$ and $\nabla g(x)|_{\ker\nabla f(x)}$ are invertible (due to the maximality of their ranks); let us denote their inverses simply by $\nabla g(x)^{-1}$ and $\nabla f(x)^{-1}$.

Thus one has:

$$\begin{array}{lcl} \nabla g(x)^{-1}\nabla g(x) = \pi_f(x) & \text{and} & \nabla g(x)\nabla g(x)^{-1} = \mathbb{1}_{p\times p} \\ \nabla f(x)^{-1}\nabla f(x) = \pi_g(x) & & \nabla f(x)\nabla f(x)^{-1} = \mathbb{1}_{d-p\times d-p}. \end{array} \tag{4.1.1}$$

It follows that $\nabla\phi(x)$ can be inverted in terms of $\nabla g(x)^{-1}$ and $\nabla f(x)^{-1}$; its inverse is

$$\nabla\phi(x)^{-1} = \left[\,\nabla g(x)^{-1}\;\;\nabla f(x)^{-1}\,\right].$$

Analogously, ${}^t\nabla g(x)$ and ${}^t\nabla f(x)$ are invertible as soon as their counter-domains are restricted to $(\ker\nabla g(x))^\perp$ and $(\ker\nabla f(x))^\perp$ (in which case the transpose of the relations in (4.1.1) hold), allowing us to write the coordinate transformation in cotangent space as:

$$\begin{array}{rcl} \zeta & = & {}^t\nabla\phi\,(x)^{-1}\,\xi \\ \left(\begin{array}{c} \zeta' \\ \zeta'' \end{array}\right) & = & \left[\begin{array}{c} {}^t\nabla g(x)^{-1}\,{}^t\pi_f(x) \\ {}^t\nabla f(x)^{-1}\,{}^t\pi_g(x) \end{array}\right]\xi. \end{array} \tag{4.1.2}$$

Geometrically, let be the manifold $\Lambda = \{x \in \mathbb{R}^d : g(x) = 0\}$, parametrized locally by the variable $z'' \in \mathbb{R}^{d-p}$. For a $x \in \Lambda$, the cotangent space can be described by $T_x^*\Lambda = \ker\nabla g(x)$ (see Remark 3.1.1) and its elements are parametrized by ζ''. The variables z' and ζ' in $\mathbb{R}^p$ will be associated with the normal and conormal spaces $N_x\Lambda = \mathbb{R}^d/T_x\Lambda$ and $N_x^*\Lambda = \mathbb{R}^d/T_x^*\Lambda$. We will also be using variables $\omega = \frac{z'}{\|z'\|}$ for $z' \neq 0$, which will be identified as elements of the normal space in sphere of Λ, $S_x\Lambda = N_x\Lambda/\mathbb{R}_*^+$.

Remark 4.1.1. Due to the fact that the coordinate z' is defined equally in any local charts by $z' = g(x)$, one can define functions on $\mathbb{R}^p$, more specifically on $N_x\Lambda$, simply by its explicit formulation in z'; further, Λ not being empty allows us to always calculate a function at $z' = 0$. These facts are implicitly used in the calculations to come.

At this point we shall state a central result in semiclassical analysis (see for instance Proposition 5.1 of [9] and its proof):

Proposition 4.1.2. *Let be ϕ a diffeomorphism of $\mathbb{R}^d$ in the sense of manifolds, and $\tilde{\phi}$ the correspondent cotangent bundle transformation, $\tilde{\phi}(x,\xi) = \left(\phi(x), {}^t\nabla\phi(x)^{-1}\xi\right)$. Let $T_\phi \in$*

$\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$ *be the operator such that* $T_\phi f = \left(J_\phi \circ \phi^{-1}\right)^{-\frac{1}{2}} f \circ \phi^{-1}$*, where* J_ϕ *is the Jacobian of* ϕ*. Then,* $T_\phi^* T_\phi = \mathbb{1}$ *and*

$$\langle \operatorname{op}_\varepsilon(a)\, \Psi_t^\varepsilon, \Psi_t^\varepsilon \rangle = \left\langle \operatorname{op}_\varepsilon(a \circ \tilde{\phi}^{-1})\, T_\phi \Psi_t^\varepsilon \,,\, T_\phi \Psi_t^\varepsilon \right\rangle + \varepsilon \sup_{\substack{\alpha,\beta \in \mathbb{N}_0^d \\ |\alpha|+|\beta|=1}} N_{d+1}\left(\partial_x^\alpha \partial_\xi^\beta a\right),$$

where $N_{d+1}(a)$ *is the upper bound in* (2.1.3)*.*

Besides, denoting $\psi_t^\varepsilon = T_\phi \Psi_t^\varepsilon$ *and* $\tilde{V} = V \circ \phi^{-1}$*, the local expression for* ψ_t^ε *satisfies the equation*

$$i\varepsilon \partial_t \psi_t^\varepsilon(x) = -\frac{\varepsilon^2}{2} T_\phi \Delta T_\phi^* \,\psi_t^\varepsilon(x) + \tilde{V}(x)\, \psi_t^\varepsilon(x). \tag{4.1.3}$$

As a consequence, if $\tilde{\mu}$ is the measure associated to the family $(\psi^\varepsilon)_{\varepsilon>0}$, for any symbol $a \in C_0^\infty(\mathbb{R}^{2d})$ and $\Xi \in C_0^\infty(\mathbb{R})$, one has

$$\langle \mu \,,\, \Xi\, a \rangle_{\mathbb{R}\times\mathbb{R}^{2d}} = \left\langle \tilde{\mu} \,,\, \Xi\, a \circ \tilde{\phi}^{-1} \right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}},$$

i.e, any result got for the new measure $\tilde{\mu}$ can be immediately transferred to the original μ by simply changing the coordinate system. Analogous arguments and some more work result in a similar statement for the two-microlocal measures. Noting $\mathcal{M}(V)$ the set of measures over the locally convex space V, we get:

Corollary 4.1.3. *Geometrically, the Wigner and the two-microlocal measures to be built ahead will be* $\mu \in \mathcal{M}\left(\mathbb{R} \times \mathbb{R}^{2d}\right)$*,* $\mathfrak{m} \in \mathcal{M}\left(\mathbb{R} \times E\Lambda\right)$ *and* $\nu_\infty \in \mathcal{M}\left(\mathbb{R} \times SE\Lambda\right)$*, where the bundles* $E\Lambda$ *and* $SE\Lambda$ *have fibres*

$$E_\sigma\Lambda = T_\sigma^*\Lambda \oplus N_\sigma^*\Lambda \oplus N_\sigma\Lambda$$

and

$$SE_\sigma\Lambda = T_\sigma^*\Lambda \oplus N_\sigma^*\Lambda \oplus S_\sigma\Lambda.$$

Proof. See the proof of Corollary 9.4.3 in Chapter 9, Section 9.4, and Remark 9.4.4 in there, where we will settle in a more comfortable framework. ☐

Therefore, Theorem 3.2.1 will follow directly from Proposition 4.5.6 and a trivial application of Corollary 4.1.3.

Remark 4.1.4. Since in the rest of this work the variables that we will write are going to be dummy, we will not care about marking the differences between (x, ξ) and (z, ζ), nor about keeping the notations ψ, $\tilde{\mu}$ and $\tilde{V}$ in contrast to Ψ, μ and V.

In short, now we can fairly relay on the study of the concentration of a family Ψ^ε satisfying equation (4.1.3) with a potential

$$V(x) = V_S(x) + \|x'\| F(x),$$

with $x' \in \mathbb{R}^p$, *i.e.*, satisfying the Schrödinger equation with a modified Hamiltonian operator

$$\hat{H}^\varepsilon = -\frac{\varepsilon^2}{2} T_\phi \Delta T_\phi^* + V,$$

so as that we become interested in the commutators

$$\frac{i}{\varepsilon}\left[\hat{H}^\varepsilon \,, \operatorname{op}_\varepsilon(a)\right] = \frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2} T_\phi \Delta T_\phi^* \,, \operatorname{op}_\varepsilon(a)\right] + \frac{i}{\varepsilon}\left[V_S \,, \operatorname{op}_\varepsilon(a)\right] + \frac{i}{\varepsilon}\left[\|x'\| F(x) \,, \operatorname{op}_\varepsilon(a)\right]. \tag{4.1.4}$$

In next sections we will analyse separately each one of these pieces.

4.2 The kinetic term

Let us start the computation of the first term in the right-hand side of (4.1.4) by the following exact calculation, with arbitrary $\Psi \in H^2(\mathbb{R}^d)$:

$$
\begin{aligned}
& \frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}\Delta\,,\mathrm{op}_\varepsilon(a)\right]\Psi(x) \\
= & \frac{i\varepsilon}{2(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}}\left[e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}a\left(\frac{x+y}{2},\xi\right)\Delta_y\Psi(y)-\Delta_x\left(e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}a\left(\frac{x+y}{2},\xi\right)\right)\Psi(y)\right]d\xi dy \\
= & \frac{i\varepsilon}{2(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}}(\Delta_y-\Delta_x)\left(e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}a\left(\frac{x+y}{2},\xi\right)\right)\Psi(y)\,d\xi dy \\
= & \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}}e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}\xi\cdot\partial_x a\left(\frac{x+y}{2},\xi\right)\Psi(y)\,d\xi dy \\
= & \mathrm{op}_\varepsilon\left(\xi\cdot\partial_x a(x,\xi)\right)\Psi(x).
\end{aligned}
$$

Observe that $\xi\cdot\partial_x a \in C_0^\infty(\mathbb{R}^{2d})$, thus the pseudodifferential operator above can be extended to $L^2(\mathbb{R}^d)$, where it will be uniformly bounded with respect to ε. Moreover, using last identity,

$$
\begin{aligned}
\frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}T_\phi\,\Delta\,T_\phi^*\,,\,\mathrm{op}_\varepsilon(a)\right] &= T_\phi\frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}\Delta\,,\,T_\phi^*\,\mathrm{op}_\varepsilon(a)\,T_\phi\right]T_\phi^* \\
&= T_\phi\frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}\Delta\,,\,\mathrm{op}_\varepsilon\left(a\circ\tilde{\phi}\right)\right]T_\phi^*+\mathcal{O}(\varepsilon) \\
&= T_\phi\,\mathrm{op}_\varepsilon\left(\xi\cdot\partial_x\left(a\circ\tilde{\phi}\right)\right)T_\phi^*+\mathcal{O}(\varepsilon) \\
&= \mathrm{op}_\varepsilon\left(\left(\xi\cdot\partial_x\left(a\circ\tilde{\phi}\right)\right)\circ\tilde{\phi}^{-1}\right)+\mathcal{O}(\varepsilon) \\
&= \mathrm{op}_\varepsilon\left(D(x)\xi\cdot\partial_x a\right)+\mathcal{O}(\varepsilon)\,,
\end{aligned}
$$

where $D(x)=\nabla\phi\left(\phi^{-1}(x)\right)^t\,\nabla\phi\left(\phi^{-1}(x)\right)$ reads:

$$
D(x)=\begin{bmatrix}\nabla g\left(\phi^{-1}(x)\right)\\ \nabla f\left(\phi^{-1}(x)\right)\end{bmatrix}\begin{bmatrix}{}^t\nabla g\left(\phi^{-1}(x)\right) & {}^t\nabla f\left(\phi^{-1}(x)\right)\end{bmatrix}.
$$

The result is:

$$
\begin{aligned}
&\int_{\mathbb{R}}\Xi(t)\left\langle\frac{i}{\varepsilon}\left[-\frac{\varepsilon^2}{2}\Delta\,,\mathrm{op}_\varepsilon(a)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle dt \\
&\underset{\varepsilon\to 0}{\longrightarrow}\; -\left\langle D(x)\xi\cdot\partial_x\mu(t,x,\xi)\,,\Xi(t)\,a(x,\xi)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}\,.
\end{aligned}
\tag{4.2.1}
$$

Remark 4.2.1. Observe that $(D(x)\xi)'=\nabla g\left(\phi^{-1}(x)\right)^t\,\nabla\phi\left(\phi^{-1}(x)\right)\xi$ and $(D(x)\xi)''=\nabla f\left(\phi^{-1}(x)\right)^t\,\nabla\phi\left(\phi^{-1}(x)\right)\xi$. Back to the original coordinates, this gives $(D(z)\zeta)'=\nabla g(x)\xi$ and $(D(z)\zeta)''=\nabla f(x)\xi$. Besides, from (4.1.2) we have $\zeta'={}^t\nabla g(x)^{-1}\,{}^t\pi_f(x)\xi$ and $\zeta''={}^t\nabla f(x)^{-1}\,{}^t\pi_g(x)\xi$, which implies

$$
\nabla g(x)^t\nabla f(x)\zeta''=\nabla g(x)\,{}^t\pi_g(x)\xi \quad\text{and}\quad \nabla f(x)^t\nabla g(x)\zeta'=\nabla f(x)^t\pi_f(x)\xi;
$$

as we chose f so as to have $\pi_g(x)$ and $\pi_f(x)$ orthogonal when $x\in\Lambda$, we are left with $D(0,z'')\zeta=(D_g(0,z'')\zeta'\,,\,D_f(0,z'')\zeta'')$, where $D_g(z)=\nabla g\left(\phi^{-1}(z)\right)^t\,\nabla g\left(\phi^{-1}(z)\right)$ is invertible for $z=(0,z'')$ and the same for $D_f(z)$ analogously defined.

4.3 The dynamical term – smooth part

Consider the Taylor developments

$$V_S(x) = V_S\left(\frac{x+y}{2}\right) + \frac{1}{2}\int_0^1 \nabla V_S\left(\frac{x+y}{2} + s\frac{x-y}{2}\right) \cdot (x-y)ds$$

and

$$\nabla V_S\left(\frac{x+y}{2} + s\frac{x-y}{2}\right) = \nabla V_S\left(\frac{x+y}{2}\right) + \frac{1}{2}\int_0^1 \nabla^2 V_S\left(\frac{x+y}{2} + s's\frac{x-y}{2}\right) \cdot (x-y)ds';$$

plugging the latter inside the former[2] and subtracting the resulting formula from the development one would obtain doing the same for $V_S(y)$ centred around $\frac{x+y}{2}$, we get:

$$\begin{aligned} V_S(x) - V_S(y) = \nabla V_S\left(\frac{x+y}{2}\right) \cdot (x-y) + \frac{1}{4}\int_0^1\int_0^1 s\left(\nabla^2 V_S\left(\frac{x+y}{2} + s's\frac{x-y}{2}\right)\right. \\ \left. -\nabla^2 V_S\left(\frac{x+y}{2} - s's\frac{x-y}{2}\right)\right)(x-y)^{(2)}\, ds'ds. \end{aligned} \tag{4.3.1}$$

Now, consider also the fact that $\frac{i}{\varepsilon}\left[\, V_S\,, \mathrm{op}_\varepsilon(a)\,\right]$ has kernel

$$k(x,y) = \frac{i}{\varepsilon^{d+1}}\mathcal{F}_\xi^{-1}a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)(V_S(x) - V_S(y))\,. \tag{4.3.2}$$

Since so far we are still dealing with smooth symbols, as in standard symbolic calculus we use the formula $x\mathcal{F}_\xi^{-1}a = i\mathcal{F}_\xi^{-1}(\partial_\xi a)$ to exchange the factors $(x-y)$ in (4.3.1) by factors $\varepsilon\partial_\xi a$ in (4.3.2). Because both ∇V_S and $\nabla^2 V_S$ do not grow faster than some polynomial and a is compactly supported, it is a direct computation to get

$$\frac{i}{\varepsilon}\left[\, V_S\,, \mathrm{op}_\varepsilon(a)\,\right] = \mathrm{op}_\varepsilon\left(-\nabla V_S \cdot \partial_\xi a\right) + \mathcal{O}\left(\varepsilon\right),$$

where $\mathcal{O}(\varepsilon)$ tends to 0 in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$ and $\mathrm{op}_\varepsilon(-\nabla V_S \cdot \partial_\xi a)$ is uniformly bounded with respect to ε. This naturally gives

$$\begin{aligned} &\int_{\mathbb{R}} \Xi(t)\left\langle \frac{i}{\varepsilon}\left[\, V_S\,, \mathrm{op}_\varepsilon(a)\,\right]\Psi_t^\varepsilon\,, \Psi_t^\varepsilon \right\rangle dt \\ &\qquad \underset{\varepsilon\to 0}{\longrightarrow} \;\left\langle\, \nabla V_S(x) \cdot \partial_\xi \mu(t,x,\xi)\,, \Xi(t)\, a(x,\xi)\,\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}. \end{aligned} \tag{4.3.3}$$

4.4 The dynamical term – singular part

In order to analyse the commutator with $\|x'\|F$ in (4.1.4), we will introduce a cut-off $\chi \in C_0^\infty(\mathbb{R}^p)$, $0 \leqslant \chi \leqslant 1$, $\chi(x') = 0$ for $\|x'\| \geqslant 1$ and $\chi(x') = 1$ for $\|x'\| \leqslant \frac{1}{2}$. Let us cut the symbol a into three parts using parameters $R > 0$ and $\delta > \varepsilon R$, as follows:

$$a(x,\xi) = a(x,\xi)\,\chi\left(\frac{x'}{\varepsilon R}\right) + a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right) + a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right). \tag{4.4.1}$$

In the context of two-microlocal analysis, each of these pieces is related to a different two-microlocal measure, and that is what we will be talking about in the next sections.

[2] This kind of procedure will be largely used in the following pages, but we will not repeat the calculations textually everytime; exposing the kernels issued from the second order terms will be sufficient for our analyses.

4.4.1 The inner part

Defining $\tilde{\Psi}^\varepsilon(x) = \varepsilon^{\frac{p}{2}}\Psi^\varepsilon(\varepsilon x', x'')$, one calculates:

$$
\begin{aligned}
&\left\langle \frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\mathrm{op}_\varepsilon\left(a(x,\xi)\chi\left(\frac{x'}{\varepsilon R}\right)\right)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle \\
=\; & \frac{i}{\varepsilon\,(2\pi\varepsilon)^d}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}\,a\left(\frac{x+y}{2},\xi\right)\chi\left(\frac{x'+y'}{2\varepsilon R}\right)\left(\|x'\|F(x)-\|y'\|F(y)\right) \\
& \qquad \Psi_t^\varepsilon\,(y)\,\overline{\Psi_t^\varepsilon\,(x)}\,dxd\xi dy \\
=\; & \int_{\mathbb{R}^{3d}} \frac{ie^{i\xi'\cdot(x'-y')}e^{\frac{i}{\varepsilon}\xi''\cdot(x''-y'')}}{(2\pi)^d\,\varepsilon^{d-p}}\,a\left(\varepsilon\frac{x'+y'}{2},\frac{x''+y''}{2},\xi',\xi''\right)\chi\left(\frac{x'+y'}{2R}\right) \\
& \qquad \left(\|x'\|F(\varepsilon x',x'')-\|y'\|F(\varepsilon y',y'')\right)\tilde{\Psi}_t^\varepsilon\,(y)\,\overline{\tilde{\Psi}_t^\varepsilon\,(x)}\,dxd\xi dy \\
=\; & \int_{\mathbb{R}^{3d}} \frac{ie^{i\xi'\cdot(x'-y')}e^{\frac{i}{\varepsilon}\xi''\cdot(x''-y'')}}{(2\pi)^d\,\varepsilon^{d-p}}\,a\left(0,\frac{x''+y''}{2},\xi',\xi''\right) \\
& \qquad \chi\left(\frac{x'+y'}{2R}\right)F\left(0,\frac{x''+y''}{2}\right)\left(\|x'\|-\|y'\|\right)\tilde{\Psi}_t^\varepsilon\,(y)\,\overline{\tilde{\Psi}_t^\varepsilon\,(x)}\,dxd\xi dy + R^\varepsilon,
\end{aligned}
\tag{4.4.2}
$$

with R^ε an error of order ε in $\mathbb{R}$ whose analysis will be postponed.

Now, for each $x'',\xi''\in\mathbb{R}^{d-p}$, denote by

$$
kA^R_{(x'',\xi'')}\,(x',y') = \frac{i}{(2\pi)^p}\int_{\mathbb{R}^p} e^{i\xi'\cdot(x'-y')}a\,(0,x'',\xi',\xi'')\,\chi\left(\frac{x'+y'}{2R}\right)\left(\|x'\|-\|y'\|\right)F\,(0,x'')\,d\xi'
$$

the integral kernel of the $L^2(\mathbb{R}^p_y)$ operator $A^R_{(x'',\xi'')} = i\,[\,\|y\|F(0,x'')\,,a^w_R(0,x'',\partial_y,\xi'',y)\,]$, where $a^w_R(0,x'',\partial_y,\xi'',y)$ is the Weyl quantization of the symbol $(y,\zeta)\longmapsto a(0,x'',\zeta,\xi'')\,\chi\left(\frac{y}{R}\right)$, and, as in (2.3.2), by $kU^\varepsilon_{(t,\,x'',\xi'')}$ the kernel of the correspondent bounded $L^2(\mathbb{R}^p)$ operator $U^\varepsilon_{(t,\,x'',\xi'')}$ (which is an operator-valued generalization of the Wigner transform $W^\varepsilon\Psi^\varepsilon$) introduced in Proposition 2.3.1. Then, the object in the previous calculation reads

$$
\int_{\mathbb{R}^{2d}} kA^R_{(x'',\xi'')}\,(x',y')\,kU^\varepsilon_{(t,\,x'',\xi'')}\,(y',x')\,dy'dx'dx''d\xi'' + R^\varepsilon,
$$

which gives

$$
\left\langle \frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\mathrm{op}_\varepsilon\left(a(x,\xi)\chi\left(\frac{x'}{\varepsilon R}\right)\right)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle = \mathrm{tr}\int_{\mathbb{R}^{2(d-p)}} A^R_{(x'',\xi'')}U^\varepsilon_{(t,\,x'',\xi'')}dx''d\xi''+R^\varepsilon.
$$

Regarding the error:

$$
R^\varepsilon = i\varepsilon\left\langle\left(B^\varepsilon + C^\varepsilon\right)\tilde{\Psi}_t^\varepsilon\,,\tilde{\Psi}_t^\varepsilon\right\rangle,
$$

where B^ε and C^ε are the integral operators with the respective kernels:

$$
b^\varepsilon\,(x,y) = \frac{1}{\varepsilon^{(d-p)}}\tilde{b}^\varepsilon\left(\frac{x+y}{2},x'-y',\frac{x''-y''}{\varepsilon}\right)
$$

and

$$
c^\varepsilon\,(x,y) = \frac{1}{\varepsilon^{(d-p)}}\tilde{c}^\varepsilon\left(\frac{x+y}{2},x'-y',\frac{x'-y'}{\varepsilon}\right),
$$

where one has

$$
\begin{aligned}
\tilde{b}^\varepsilon(x',x'',y',y'') = &\int_0^1 \partial_{x'}\mathcal{F}_\xi^{-1}a\,(\varepsilon s x',x'',y',y'')\cdot x'\,\chi\left(\frac{x'}{R}\right) \\
&\left(\left\|x'+\frac{y'}{2}\right\|F\left(\varepsilon\left(x'+\frac{y'}{2}\right),x''+\frac{\varepsilon y''}{2}\right)-\left\|x'-\frac{y'}{2}\right\|F\left(\varepsilon\left(x'-\frac{y'}{2}\right),x''-\frac{\varepsilon y''}{2}\right)\right)ds
\end{aligned}
$$

and

$$\tilde{c}^{\varepsilon}\left(x',x'',y'.y''\right)=\int_0^1 \mathcal{F}_{\xi}^{-1}a\left(0,x'',y',y''\right)\chi\left(\frac{x'}{R}\right)$$
$$\left[\left\|x'+\frac{y'}{2}\right\|\nabla F\left(\varepsilon s\left(x'+\frac{y'}{2}\right),x''+s\frac{\varepsilon y''}{2}\right)\cdot\left(x'+\frac{y'}{2},\frac{y''}{2}\right)\right.$$
$$\left.+\left\|x'-\frac{y'}{2}\right\|\nabla F\left(\varepsilon s\left(x'-\frac{y'}{2}\right),x''-s\frac{\varepsilon y''}{2}\right)\cdot\left(x'-\frac{y'}{2},\frac{y''}{2}\right)\right]ds.$$

Lemma 4.4.1. *The operators B^{ε} and C^{ε} are uniformly bounded with respect to ε.*

Proof. Let us prove the lemma for B^{ε} by using the conventional Schur test and the fact that $\mathcal{F}_{\xi}^{-1}a$ is a rapidly decreasing function bounded by the polynomial $\mathfrak{p}$ given in the beginning of Section 3.1).

In fact, noting $\mathfrak{P}=\max_{\|x'\|\leqslant R}\mathfrak{p}(x',0)$ and recalling the sub-additivity of $\mathfrak{p}$, we have some $K\geqslant 1$ such that

$$\left|\tilde{b}^{\varepsilon}(x,y)\right|\ \leqslant\ \mathbb{1}_{\{\|x'\|\leqslant R\}}\left(R+\frac{\|y'\|}{2}\right)K\left(\mathfrak{P}+\mathfrak{p}(0,x'')+\mathfrak{p}(\varepsilon y)\right)\max_{\substack{z\in\mathbb{R}^p\\ \|z\|\leqslant R}}\left\|\partial_{x'}\mathcal{F}_{\xi}^{-1}a(z,x'',y)\right\|_{\mathcal{L}(\mathbb{R}^p)},$$

which shows that $\tilde{b}^{\varepsilon}$ is also a Schwartz function, implying:

$$\begin{aligned}
\sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}\left|b^{\varepsilon}(x,y)\right|dy &\leqslant \sup_{x\in\mathbb{R}^d}\frac{1}{\varepsilon^{(d-p)}}\int_{\mathbb{R}^d}\left|\tilde{b}^{\varepsilon}\left(\frac{x+y}{2},x'-y',\frac{x''-y''}{\varepsilon}\right)\right|dy\\
&= \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}\left|\tilde{b}^{\varepsilon}\left(x'-\frac{y'}{2},x''-\frac{\varepsilon y''}{2},y',y''\right)\right|dy\\
&= \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}\left|\tilde{b}^{\varepsilon}\left(x'-\frac{y'}{2},x''-\frac{\varepsilon y''}{2},y\right)\langle y\rangle^{2d}\right|\langle y\rangle^{-2d}dy\\
&\leqslant \max_{x,y\in\mathbb{R}^d}\left|\tilde{b}^{\varepsilon}\left(x,y\right)\langle y\rangle^{2d}\right|\int_{\mathbb{R}^d}\langle y\rangle^{-2d}dy\\
&< \infty.
\end{aligned}$$

The estimate $\sup_{y\in\mathbb{R}^d}\int_{\mathbb{R}^d}|b^{\varepsilon}(x,y)|<\infty$ is found by following the very same steps above, so Schur's lemma allows us to conclude that $\|B^{\varepsilon}\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)}<\infty$ uniformly with respect to ε.

Regarding C^{ε}, the proof is, *mutatis mutandis*, exactly as we have done for B^{ε} and will be omitted. □

Now we only need to focus on the lasting term; from what we have seen in Section 2.3, in the limit where $\varepsilon\longrightarrow 0$ and then $R\longrightarrow\infty$, it gives

$$\int_{\mathbb{R}}\Xi(t)\left\langle\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\mathrm{op}_{\varepsilon}\left(a(x,\xi)\chi\left(\frac{x'}{\varepsilon R}\right)\right)\right]\Psi_t^{\varepsilon}\,,\Psi_t^{\varepsilon}\right\rangle dt$$
$$\longrightarrow\quad \mathrm{tr}\left\langle M\left(t,x'',\xi''\right)\,,\,i\left[\,\|y\|F\left(0,x''\right),\Xi(t)\,a^{w}\left(0,x'',\partial_y,\xi''\right)\right]\right\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}},\tag{4.4.3}$$

where M is the two-microlocal operator-valued measure in Proposition 2.3.1.

In Section 4.5, M will be shown to be zero; for now, let us prove:

Lemma 4.4.2. *One has got the estimate*

$$\operatorname{tr}\left\langle M\left(t,x'',\xi''\right)\,,\,i\left[\,\|y\|F\left(0,x''\right),\Xi(t)\,a^{w}\left(0,x'',\partial_y,\xi''\right)\,\right]\right\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}}$$

$$\leqslant TK\sup_{\substack{\alpha\in\mathbb{N}_0^d\\|\alpha|\leqslant d+1}}\sup_{x''\in\mathbb{R}^{d-p}}\int_{\mathbb{R}^d}\left\|\partial_\xi^\alpha\partial_{\xi'}a(0,x'',\xi)F(0,x'')\right\|_{\mathbb{R}^p}d\xi, \tag{4.4.4}$$

where $T,K>0$ are constants, $\Xi\in C_0^\infty([-T,T])$ and $a\in C_0^\infty(\mathbb{R}^{2d})$.

Proof. From a calculation similar to that we made in (4.4.2) and similar estimates, it follows that

$$\left\langle\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\operatorname{op}_\varepsilon\left(a(x,\xi)\chi\left(\frac{x'}{\varepsilon R}\right)\right)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle=\left\langle P^\varepsilon\,\tilde\Psi_t^\varepsilon\,,\,\tilde\Psi_t^\varepsilon\right\rangle+\mathcal{O}(\varepsilon),$$

where P^ε is the operator with kernel

$$\begin{aligned}p^\varepsilon(x,y)&=\int_{\mathbb{R}^d}\frac{ie^{i\xi\cdot(x-y)}}{(2\pi)^d}a\left(0,\frac{x''+y''}{2},\xi',\varepsilon\xi''\right)\chi\left(\frac{x'+y'}{2R}\right)F(0,x'')\left(\|x'\|-\|y'\|\right)d\xi\\&=-\int_{\mathbb{R}^d}\frac{e^{i\xi\cdot(x-y)}}{(2\pi)^d}\frac{x'+y'}{\|x'\|+\|y'\|}\cdot\partial_{\xi'}a\left(0,\frac{x''+y''}{2},\xi',\varepsilon\xi''\right)\chi\left(\frac{x'+y'}{2R}\right)F(0,x'')d\xi\end{aligned}$$

(recall: $\|x'\|-\|y'\|=\frac{x'+y'}{\|x'\|+\|y'\|}\cdot(x'-y')$). Further, let be $\tilde b$ the kernel of the operator $\operatorname{op}_{1,\varepsilon}(b)=\operatorname{op}_1\left(b(x,\xi',\varepsilon\xi'')\right)$, with

$$b(x,\xi)=-\mathbf{1}_p\cdot\partial_\xi a(0,x'',\xi)\,\chi\left(\frac{x'}{R}\right)F(0,x''),$$

where $\mathbf{1}_p=(1,\dots,1)\oplus(0,\dots,0)\in\mathbb{R}^p\times\mathbb{R}^{d-p}$.

Observe that $|p^\varepsilon(x,y)|\leqslant|\tilde b(x,y)|$, which causes the Schur estimate for the norm of $\operatorname{op}_{1,\varepsilon}(b)$ to be greater than that for P^ε. Besides, the Schur estimate for $\operatorname{op}_{1,\varepsilon}(b)$ is upper bounded by an estimate of type (2.1.3) (see Remark 2.1.1), which must, consequently, be an upper bound for the norm of P^ε as well. This estimate is the one we stated in the lemma. □

Remark 4.4.3. In [45], an estimate that turns up to be equivalent to last lemma was obtained by noticing directly that $\frac{i}{\varepsilon}\left[\|x'\|F(x),\operatorname{op}_\varepsilon(a)\right]$ is bounded uniformly with respect to ε, which was used in proving that $\frac{i}{\varepsilon}\left[\hat H^\varepsilon,\operatorname{op}_\varepsilon(a)\right]$ is itself bounded.

4.4.2 The outer part

We start by proving with standard symbolic calculus the technical result below:

Lemma 4.4.4. *For $\delta>0$, $\delta\geqslant\varepsilon R$, one has the following estimation in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$:*

$$\begin{aligned}\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\operatorname{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\right]&=\frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right),\operatorname{op}_\varepsilon\left(a(x,\xi)\right)\right]\\&\quad-\operatorname{op}_\varepsilon\left(\frac{1}{\delta}\|x'\|F(x)\,\chi'\left(\frac{x'}{\delta}\right)\cdot\partial_{\xi'}a(x,\xi)\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right).\end{aligned}$$

Proof. In view of the identities

$$\begin{aligned}\operatorname{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)&=\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\operatorname{op}_\varepsilon\left(a(x,\xi)\right)+R^l_{\varepsilon,\delta}\\&=\operatorname{op}_\varepsilon\left(a(x,\xi)\right)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)+R^r_{\varepsilon,\delta},\end{aligned}$$

where $R^l_{\varepsilon,\delta}$ and $R^r_{\varepsilon,\delta}$ have integral kernels

$$r^l_{\varepsilon,\delta}(x,y) = \frac{i}{\varepsilon^d}\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\left(\chi\left(\frac{x'}{\delta}\right) - \chi\left(\frac{x'+y'}{2\delta}\right)\right)$$

and

$$r^r_{\varepsilon,\delta}(x,y) = \frac{i}{\varepsilon^d}\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\left(\chi\left(\frac{y'}{\delta}\right) - \chi\left(\frac{x'+y'}{2\delta}\right)\right),$$

we have

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\right] = \frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\,,\mathrm{op}_\varepsilon\left(a(x,\xi)\right)\right] + \underbrace{\frac{i}{\varepsilon}\left(\|x'\|F(x)R^l_{\varepsilon,\delta} - R^r_{\varepsilon,\delta}\|x'\|F(x)\right)}_{R_{\varepsilon,\delta}},$$

where $R_{\varepsilon,\delta}$ has kernel

$$r_{\varepsilon,\delta}(x,y) = \frac{i}{\varepsilon^{d+1}}\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\left(\chi\left(\frac{x'}{\delta}\right)\|x'\|F(x) - \chi\left(\frac{y'}{\delta}\right)\|y'\|F(y) - \chi\left(\frac{x'+y'}{2\delta}\right)\left(\|x'\|F(x) - \|y'\|F(y)\right)\right).$$

Using Taylor developments for χ, this kernel can be written in the form

$$r_{\varepsilon,\delta}(x,y) = \frac{i}{\varepsilon^d}\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\Bigg[\frac{1}{2\delta}\left(\|x'\|F(x) + \|y'\|F(y)\right)\chi'\left(\frac{x'+y'}{2\delta}\right)\cdot\left(\frac{x'-y'}{\varepsilon}\right)$$
$$+\frac{\varepsilon}{4\delta^2}\int_0^1\int_0^1 s\left(\chi''\left(\frac{x'+y'}{2\delta} + s's\frac{x'-y'}{2\delta}\right)\|x'\|F(x) - \chi''\left(\frac{x'+y'}{2\delta} - s's\frac{x'-y'}{2\delta}\right)\|y'\|F(y)\right)\left(\frac{x'-y'}{\varepsilon}\right)^{(2)} ds'ds\Bigg],$$

and still, with developments for $\|\cdot\|F$,

$$r_{\varepsilon,\delta}(x,y) = \frac{i}{\varepsilon^d}\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\Bigg[\frac{1}{\delta}\left\|\frac{x'+y'}{2}\right\|F\left(\frac{x+y}{2}\right)\chi'\left(\frac{x'+y'}{2\delta}\right)\cdot\left(\frac{x'-y'}{\varepsilon}\right)$$
$$+\frac{\varepsilon}{\delta}\left(\frac{x-y}{\varepsilon}\right)^{t}A(x,y)\left(\frac{x'-y'}{\varepsilon}\right) + \frac{\varepsilon}{4\delta^2}\int_0^1\int_0^1 s\left(B(x,y)\left\|\frac{x'+y'}{2}\right\|F\left(\frac{x+y}{2}\right)\right.$$
$$\left.+\varepsilon\left(\frac{x-y}{\varepsilon}\right)^{t}C(x,y)\right)\left(\frac{x'-y'}{\varepsilon}\right)^{(2)} ds'ds\Bigg],$$

where

$$A(x,y) = \frac{1}{2}\chi'\left(\frac{x'+y'}{2\delta}\right)\otimes\sum_{j=1,2}\int_0^1(-1)^j\,\nabla\left(\|\cdot\|F\right)\left(\frac{x+y}{2} + (-1)^j s''\frac{x-y}{2}\right)ds'',$$

$$B(x,y) = \sum_{j=1,2}(-1)^j\,\chi''\left(\frac{x'+y'}{2\delta} + (-1)^j s's\frac{x'-y'}{2\delta}\right)$$

and

$$C(x,y) = \frac{1}{2}\sum_{j=1,2}\int_0^1\chi''\left(\frac{x'+y'}{2\delta} + (-1)^j s's\frac{x'-y'}{2\delta}\right)\otimes\nabla\left(\|\cdot\|F\right)\left(\frac{x+y}{2} + (-1)^j s''\frac{x-y}{2}\right)ds''.$$

Observe now that A, B and C are bounded and, furthermore, B is supported on $\left\|\frac{x'+y'}{2}\right\| \leqslant \delta + \frac{\varepsilon}{2}\left\|\frac{x'-y'}{\varepsilon}\right\|$ (given that $\chi''(x')$ is null for $\|x'\| > \delta$). This, along with the identity $i\mathcal{F}_\xi^{-1}a(x,y)\,y' = -\mathcal{F}_\xi^{-1}(\partial_{\xi'}a)(x,y)$, allows us to write $R_{\varepsilon,\delta}$ as

$$R_{\varepsilon,\delta} = -\mathrm{op}_\varepsilon\left(\frac{1}{\delta}\|x'\|F(x)\,\chi'\left(\frac{x'}{\delta}\right)\cdot\partial_{\xi'}a(x,\xi)\right) + \tilde{R}_{\varepsilon,\delta},$$

where $\tilde{R}_{\varepsilon,\delta}$ has an integral kernel such that

$$|\tilde{r}_{\varepsilon,\delta}(x,y)| \leqslant \frac{Q}{\varepsilon^d}\left|\mathcal{F}_\xi a\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right)\right|\left|\frac{\varepsilon}{\delta}\left\|\frac{x-y}{\varepsilon}\right\|^2 + \frac{\varepsilon}{\delta^2}\left(\delta+\varepsilon\left\|\frac{x-y}{\varepsilon}\right\|\right)\left\|\frac{x-y}{\varepsilon}\right\|^2\right|$$

where $Q > 0$ is some constant big enough. The lemma will follow as one uses the estimation above for the Schur test to show that $\|\tilde{R}_{\varepsilon,\delta}\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leqslant \frac{\varepsilon}{\delta}$. □

Remark 4.4.5. Replacing δ by εR and $a(x,\xi)$ by $a(x,\xi)\,\chi\left(\frac{x'}{\delta}\right)$, Lemma 4.4.4 gives

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right)\right)\right] = \frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\,,\mathrm{op}_\varepsilon\left(a(x,\xi)\,\chi\left(\frac{x'}{\delta}\right)\right)\right]$$
$$-\mathrm{op}_\varepsilon\left(\frac{1}{\varepsilon R}\|x'\|F(x)\,\chi'\left(\frac{x}{\varepsilon R}\right)\boldsymbol{.}\,\partial_{\xi'}a(x,\xi)\,\chi\left(\frac{x'}{\delta}\right)\right)+\mathcal{O}\left(\frac{1}{R}\right),$$

which is going to be remarkably useful in Section 4.4.3.

Lemma 4.4.6. *For $\delta > 0$, $\delta \geqslant \varepsilon R$, one has*

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\,,\,\mathrm{op}_\varepsilon(a(x,\xi))\right] = \mathrm{op}_\varepsilon\left(-\nabla\left(\|x'\|F(x)\right)\boldsymbol{.}\,\partial_\xi a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)$$
$$+\mathrm{op}_\varepsilon\left(\frac{1}{\delta}\|x'\|F(x)\,\chi'\left(\frac{x'}{\delta}\right)\boldsymbol{.}\,\partial_{\xi'}a(x,\xi)\right)+\mathcal{O}(\varepsilon)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)$$

in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$.

Proof. Because $\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)$ is everywhere smooth, we can apply usual symbolic calculus as in 4.3.1 and 4.3.3 to get

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\,,\,\mathrm{op}_\varepsilon(a(x,\xi))\right] = \mathrm{op}_\varepsilon\left(-\partial_x\left(\|x'\|F(x)\right)\boldsymbol{.}\,\partial_\xi a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)+R^{\varepsilon,\delta}$$

where $R^{\varepsilon,\delta}$ has kernel

$$r^{\varepsilon,\delta}(x,y) = \frac{i\varepsilon}{4\varepsilon^d}\int_0^1\int_0^1 \mathcal{F}_\xi^{-1}a\left(\frac{x+y}{2},\frac{x-y}{\varepsilon}\right)B(x,y)\left(\frac{x-y}{\varepsilon}\right)^{(2)}ds'ds,$$

with B the matrix

$$B(x,y) = \sum_{j=1,2}(-1)^{-1}\,\nabla^2\left(\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\left(\frac{x+y}{2}+(-1)^j s's\frac{x-y}{2}\right).$$

From the growth properties of F, it is easy to see that there exists some $K \geqslant 1$ such that $\|B(x,y)\|_{\mathcal{L}(\mathbb{R}^d)} \leqslant K\left(\mathfrak{p}(x)+\mathfrak{p}(y)\right)\left(1+\frac{1}{\delta}\right)$ and, therefore,

$$\sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}|r(x,y)|\,dy \;\leqslant\; \varepsilon K\left(1+\frac{1}{\delta}\right)\max_{x,y\in\mathbb{R}^d}\left|\left(\mathfrak{p}(x)+\mathfrak{p}(y)\right)\mathcal{F}_\xi^{-1}a(x,y)\,y^2\,\langle y\rangle^{2d}\right|\int_{\mathbb{R}^d}\langle y\rangle^{-2d}\,dy;$$

the same estimation holding for $\sup_{y\in\mathbb{R}^d}\int_{\mathbb{R}^d}|r(x,y)|\,dx$, it follows by the Schur test that $\left\|R^{\varepsilon,\delta}\right\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \lesssim \varepsilon+\frac{\varepsilon}{\delta}$.

The rest of the proof consists on the basic derivation

$$\partial_x\left(\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\boldsymbol{.}\,\partial_\xi a(x,\xi) = \left(1-\chi\left(\frac{x'}{\delta}\right)\right)\partial_x\left(\|x'\|F(x)\right)\boldsymbol{.}\,\partial_\xi a(x,\xi)$$
$$-\frac{1}{\delta}\|x'\|F(x)\,\chi'\left(\frac{x'}{\delta}\right)\boldsymbol{.}\,\partial_{\xi'}a(x,\xi)$$

and on the linearity of the pseudodifferential operators with respect to their symbols. □

Remark 4.4.7. Analogously to Remark 4.4.5, in Section 4.4.3 we will use that

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right),\,\mathrm{op}_\varepsilon\left(a(x,\xi)\,\chi\left(\frac{x'}{\delta}\right)\right)\right]=\mathrm{op}_\varepsilon\left(-\nabla\left(\|x'\|F(x)\right)\centerdot\partial_\xi a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right)\right)$$
$$+\mathrm{op}_\varepsilon\left(\frac{1}{\varepsilon R}\|x'\|F(x)\,\chi'\left(\frac{x'}{\varepsilon R}\right)\centerdot\partial_{\xi'}a(x,\xi)\chi\left(\frac{x'}{\delta}\right)\right)+\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{1}{R}\right).$$

There, however, there will be a tiny question about the limit in ε.

Combining Lemmata 4.4.4 and 4.4.6, we obtain

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\right]=\mathrm{op}_\varepsilon\left(-\nabla\left(\|x'\|F(x)\right)\centerdot\partial_\xi a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)$$
$$+\mathcal{O}(\varepsilon)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right),$$

which gives, in the limit where $\varepsilon\longrightarrow 0$ and then $\delta\longrightarrow 0$,

$$\int_{\mathbb{R}}\Xi(t)\left\langle\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\delta}\right)\right)\right)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle dt$$
$$\longrightarrow\quad\left\langle\,\nabla\left(\|x'\|F(x)\right)\centerdot\partial_\xi\mu(t,x,\xi)\mathbb{1}_{\{x'\neq 0\}}\,,\Xi(t)\,a(x,\xi)\,\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}.\tag{4.4.5}$$

4.4.3 The middle part

As seen in Remarks 4.4.5 and 4.4.7, the calculations in Section 4.4.1 lead to

$$\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right)\right)\right]$$
$$=\quad\mathrm{op}_\varepsilon\left(-\nabla\left(\|x'\|F(x)\right)\centerdot\partial_\xi a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right)\right)+\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{1}{R}\right),$$

which implies in the two-microlocal limit when $\varepsilon\longrightarrow 0$, then $R\longrightarrow\infty$ and finally $\delta\longrightarrow 0$:

$$\int_{\mathbb{R}}\Xi(t)\left\langle\frac{i}{\varepsilon}\left[\|x'\|F(x)\,,\,\mathrm{op}_\varepsilon\left(a(x,\xi)\left(1-\chi\left(\frac{x'}{\varepsilon R}\right)\right)\chi\left(\frac{x'}{\delta}\right)\right)\right]\Psi_t^\varepsilon\,,\Psi_t^\varepsilon\right\rangle dt$$
$$\longrightarrow\quad\left\langle\delta(x')\otimes\int_{\mathcal{S}^{p-1}}F(x)\,\omega\centerdot\partial_{\xi'}\nu_\infty(t,x'',\xi,d\omega)\,,\Xi(t)\,a(x,\xi)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}},\tag{4.4.6}$$

where ν_∞ is the two-microlocal measure on sphere introduced in Proposition 2.3.1, and δ is the usual counting measure (or Dirac mass).

4.5 Establishing the equation

From equations (2.2.9), (2.2.10) and (2.2.14), more the results in the last sections, equations (4.2.1), (4.3.3), (4.4.3), (4.4.5) and (4.4.6), we obtain the equation

$$\left\langle\,\partial_t\mu+D(x)\xi\centerdot\partial_x\mu-\nabla V_S(x)\centerdot\partial_\xi\mu-\nabla\left(\|x'\|F(x)\right)\centerdot\partial_\xi\mu\mathbb{1}_{\{x'\neq 0\}}\,,\,a(t,x,\xi)\,\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}$$
$$=\left\langle\delta(x')\otimes\int_{\mathcal{S}^{p-1}}F(x)\,\omega\centerdot\partial_{\xi'}\nu_\infty(t,x'',\xi,d\omega)\,,\,a(t,x,\xi)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}$$
$$+\mathrm{tr}\left\langle\,\left[\|y\|F(0,x'')\,,M(t,x'',\xi'')\right],a^w(t,0,x'',\partial_y,\xi'')\,\right\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}}\tag{4.5.1}$$

for the full Wigner measure μ tested against a function $a\in C_0^\infty(\mathbb{R}\times\mathbb{R}^{2d})$. We will now work out this expression until we prove Proposition4.5.6 ahead.

Lemma 4.5.1. *In the two-microlocal decomposition given in Lemma 2.3.7, the operator valued measure M is zero and $\nu_\infty(t,x'',\xi,\omega)=\delta(\xi')\otimes\nu(t,x'',\xi'',\omega)$ for some measure ν on $\mathbb{R}\times\mathbb{R}^{2(d-p)}\times\mathcal{S}^{p-1}$. Consequently, equation* (4.5.1) *reads*

$$\begin{aligned}\big\langle\delta(x')\otimes\delta(\xi')\otimes\nu(t,x'',\xi'',\omega)\,,\,(\partial_t+D_f(x)\xi''\cdot\partial_{x''}-\nabla V_S(x)\cdot\partial_\xi-F(x)\,\omega\cdot\partial_{\xi'})\,a\big\rangle_{\mathbb{R}\times\mathbb{R}^{2d}\times\mathcal{S}^{p-1}}&\\ +\big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'\neq0\}}\,,(\partial_t+D(x)\xi\cdot\partial_x-\nabla V(x)\cdot\partial_\xi)\,a\big\rangle_{\mathbb{R}\times\mathbb{R}^{2d}}&\\ &=\;0\end{aligned}\tag{4.5.2}$$

for all test functions $a\in C_0^\infty(\mathbb{R}\times\mathbb{R}^{2d})$.

Remark 4.5.2. The matrix D_f above was defined in Remark 4.2.1 in analogy to D_g, also defined there. In that remark we also depicted some characteristics of this matrices that help understand the calculations ahead.

Proof. To begin with, re-write equation (4.5.1) as

$$\begin{aligned}&\big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'=0\}}\,,\,(\partial_t+D(x)\xi\cdot\partial_x-\nabla V_S(x)\cdot\partial_\xi)\,a(t,x,\xi)\,\big\rangle\\ &\quad+\big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'\neq0\}}\,,\,(\partial_t+D(x)\xi\cdot\partial_x-\nabla V(x)\cdot\partial_\xi)\,a(t,x,\xi)\,\big\rangle\\ &\qquad=\quad\Big\langle\delta(x')\otimes\int_{\mathcal{S}^{p-1}}\omega\,\nu_\infty(t,x'',\xi,d\omega)\,,\,F(x)\,\partial_\xi a(t,x,\xi)\Big\rangle\\ &\qquad\qquad-\mathrm{tr}\,\big\langle\,\big[\|y\|F(0,x'')\,,M(t,x'',\xi'')\big]\,,a^w(t,0,x'',\partial_y,\xi'')\,\big\rangle\,.\end{aligned}$$

Now, recall that the term in the trace obeys to estimate (4.4.4) given in Lemma 4.4.2; besides, since μ is a measure in $\mathcal{D}'(\mathbb{R}\times\mathbb{R}^{2d})$, we have

$$\langle\,\mu(t,x,\xi)\,,a(t,x,\xi)\,\rangle\leqslant\max_{(t,x,\xi)\in\mathbb{R}\times\mathbb{R}^{2d}}|a(t,x,\xi)|\,\mu\,(\mathrm{supp}(a))\,,\tag{4.5.3}$$

where $\mu\,(\mathrm{supp}(a))<\infty$ since μ is finite and $\mathrm{supp}(a)$, the support of a, is compact. Obviously the very same estimate (with $\mu\,(\mathrm{supp}(a))$ in the right-hand side!) is valid for $\mu(t,x,\xi)\mathbb{1}_{\{x'\neq0\}}$ and for $\delta(x')\otimes\int_{\mathcal{S}^{p-1}}\omega\,\nu_\infty(t,x'',\xi,d\omega)$. So, for test functions of the form $a_\delta(t,x,\xi)=\delta\,\theta\,(t)\,a_1\left(\frac{x'}{\delta}\right)a_2\,(x'')\,b\,(\xi)$, equation (4.5.1) gives (recalling also Remark 4.2.1):

$$\begin{aligned}&\Big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'=0\}}\,,D_g(x)\xi'\cdot\partial_{x'}a_1\left(\frac{x'}{\delta}\right)\theta\,(t)\,a_2\,(x'')\,b\,(\xi)\Big\rangle\\ &\qquad+\Big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'\neq0\}}\,,(D(x)\xi)'\cdot\partial_{x'}a_1\left(\frac{x'}{\delta}\right)\theta\,(t)\,a_2\,(x'')\,b\,(\xi)\Big\rangle+\mathcal{O}(\delta)=0,\end{aligned}$$

that at the limit where $\delta\longrightarrow0$ results in

$$\partial_{x'}a_1(0)\cdot\big\langle\mu(t,x,\xi)\mathbb{1}_{\{x'=0\}}\,,D_g(0,x'')\xi'\,\theta(t)\,a_2(x'')\,b(\xi)\big\rangle=0,$$

which means that $\mu(t,x,\xi)\mathbb{1}_{\{x'=0\}}$ is supported on $\mathbb{R}\times\{\xi'=0\}\times\mathbb{R}^{2d-p}_{x,\xi''}$, and, by positivity, ν_∞ is necessarily supported on $\mathbb{R}\times\{\xi'=0\}\times\mathbb{R}^{2(d-p)}_{x'',\xi''}\times\mathcal{S}^{p-1}$ and the measure $\mathfrak{m}$ introduced in Remark 2.3.3 in $\mathbb{R}\times\{\xi'=0\}\times\mathbb{R}^{2d-p}_{x'',\xi'',\rho}$.

Regarding ν_∞, any measure supported on $\xi'=0$ can only be a Dirac mass thereon[3], whence there must be ν as stated in the Lemma. However, for $\mathfrak{m}$ we already knew that it was

[3]More generally, a distribution supported on such a set can be developed as $\sum_{n\in\mathbb{N}_0}c_n\delta^{(n)}(\xi')$, where $c_n\in\mathbb{C}$ and $\delta^{(n)}$ is the n-th distribution derivative of the Dirac δ. As our distribution must be a positive measure as well, the only allowed term in this development is the one with $n=0$.

absolutely continuous with respect to $d\xi'$ (Lemma 2.3.5), so being zero almost everywhere in ξ' is, in other words, saying that $\mathfrak{m} = 0$. From Lemma 2.3.4, this implies that $M = 0$ and, finally, that so is the term in the trace in equation (4.5.1).

To conclude, just re-write (4.5.1) attaching all the information we have just got and verify that it simplifies to (4.5.2). □

Remark 4.5.3. As a scholium of the last proof, one has that μ is not supported on the region of the ξ' axis away from the origin, $\{(0,\xi') \in \mathbb{R}^{2p} : \xi' \neq 0\}$. This implies that $\mu(t,x,\xi)\mathbb{1}_{\{x'\neq 0\}} = \mu(t,x,\xi)\mathbb{1}_{\{(x',\xi')\neq(0,0)\}}$, which is a result that [45] had already obtained with a similar argument.

Lemma 4.5.4. *One has the identity* $\nabla_{x'} V(x)\, \mathbb{1}_{\{x'\neq 0\}} \mathbb{1}_{\{\xi'=0\}} \mu(t,x,\xi) = 0$.

Proof. Recall estimate (4.5.3), which holds for $\mu(t,x,\xi)\mathbb{1}_{\{x'\neq 0\}}$ and for $\delta(x') \otimes \nu_\infty(t,x'',\xi,\omega)$ as well. Thus, for test functions of the form $a_\delta(t,x,\xi) = \delta\, \theta(t)\, (x')^2\, a(x)\, b_1\left(\frac{\xi'}{\delta}\right) b_2(\xi)$ and proceeding in the same manner as in the proof of Lemma 4.5.1, equation (4.5.2) gives, in the limit where $\delta \longrightarrow 0$,

$$\partial_{\xi'} b_1(0) \,.\, \left\langle\, \nabla_{x'} V(x)\, \mathbb{1}_{\{x'\neq 0\}} \mathbb{1}_{\{\xi'=0\}} \mu(t,x,\xi)\, , (x')^2\, \theta(t)\, a(x)\, b_2(\xi) \,\right\rangle = 0,$$

which means that the distribution $\nabla_{x'} V(x)\, \mathbb{1}_{\{x'\neq 0\}} \mathbb{1}_{\{\xi'=0\}} \mu(t,x,\xi)$ is supported on $\mathbb{R} \times \{x' = 0\} \times \mathbb{R}^{2d-p}_{x'',\xi}$. But of course this carries that it is null. □

Lemma 4.5.5. *The measure ν introduced in Lemma 4.5.1 obeys to the following identity in the sense of the distributions on* $\mathbb{R} \times \mathbb{R}^{2(d-p)}_{x'',\xi''}$*:*

$$\int_{\mathcal{S}^{p-1}} \big(\nabla_{x'} V_S(0,x'') + F(0,x'')\, \omega\big)\, \nu(t,x'',\xi'',d\omega) = 0,$$

where V_S and F are as in (3.1.4).

Proof. For test functions of the form $a_\delta(t,x,\xi) = \delta\, \theta(t)\, a(x)\, b_1\left(\frac{\xi'}{\delta}\right) b_2(\xi'')$, using estimate (4.5.3) and Lemma 4.5.4, the present lemma follows from (4.5.2) at the limit $\delta \longrightarrow 0$. □

To finish establishing a Liouville equation for μ, let us put all Lemmata 4.5.1, 4.5.4, 4.5.5 and Remark 4.2.1 together and write equation (4.5.2) in a distributional and clearer way:

$$\begin{aligned} \delta(x') \otimes \delta(\xi') \otimes \int_{\mathcal{S}^{p-1}} (\partial_t + D_f(x)\xi'' \,.\, \partial_{x''} - \nabla_{x''} V_S(0,x'') \,.\, \partial_{\xi''})\, \nu(t,x'',\xi'',d\omega) & \\ + (\partial_t + D(x)\xi \,.\, \partial_x - \nabla V(x) \,.\, \partial_\xi)\, \mu(t,x,\xi)\mathbb{1}_{\{x'\neq 0\}} &= 0, \end{aligned}$$

or, more explicitly, in view of Remark 4.5.3:

Proposition 4.5.6. *Let be $V(x) = V_S(x) + \|x'\| F(x)$ a conical potential with $x' \in \mathbb{R}^p$, $1 \leqslant p \leqslant d$, $x = (x',x'')$. Let be Ψ^ε the solution to the Schrödinger equation* (3.1.2) *with potential V. Then, the Wigner measure associated to the concentration of Ψ^ε in the limit $\varepsilon \longrightarrow 0$ can be decomposed as*

$$\mu(t,x,\xi) = \mathbb{1}_{\{(x',\xi')\neq(0,0)\}} \mu(t,x,\xi) + \delta(x') \otimes \delta(\xi') \otimes \int_{\mathcal{S}^{p-1}} \nu(t,x'',\xi'',d\omega),$$

where the measure ν satisfies the asymmetry condition

$$\int_{\mathcal{S}^{p-1}} \left(\nabla_{x'} V_S(0,x'') + F(0,x'')\,\omega\right) \nu(t,x'',\xi'',d\omega) = 0.$$

Besides, it obeys to the following distributional equation in $\mathcal{D}'(\mathbb{R}\times\mathbb{R}^{2d})$:

$$\begin{aligned}\left(\partial_t + (D(x)\xi)'' \cdot \partial_{x''} - \nabla_{x''} V_S(0,x'') \cdot \partial_{\xi''}\right) \left(\mu(t,x,\xi) 1\!\!1_{\{(x',\xi')=(0,0)\}}\right) \\ + \left(\partial_t + D(x)\xi \cdot \partial_x - \nabla V(x) \cdot \partial_\xi\right) \left(\mu(t,x,\xi) 1\!\!1_{\{(x',\xi')\neq(0,0)\}}\right) &= 0,\end{aligned}$$

where $D(x) = \nabla\phi\left(\phi^{-1}(x)\right)^t \nabla\phi\left(\phi^{-1}(x)\right)$.

4.6 Continuity in t and absolute continuity with respect to dt

From equation (2.2.8), it is obvious that μ is absolutely continuous with respect to the Lebesgue measure dt, which implies the existence of a function $\mathbb{R} \ni t \longmapsto \mu_t$ taking values in the set of positive measures on $\mathbb{R}^{2d}$ such that $\mu(t,x,\xi) = \mu_t(x,\xi)dt$. The same holds for the two-microlocal measure ν, since it is positive and absolutely continuous with respect to μ, carrying the existence of a function $t \longmapsto \nu_t$ such that $\nu(t,x'',\xi'',\omega) = \nu_t(x'',\xi'',\omega)dt$.

Nevertheless, the same is not true for continuity. In fact, in [45] it was shown that $t \longmapsto \mu_t$ is continuous inside a compact $[-T,T]$ by verifying that, for $a \in C_0^\infty(\mathbb{R}^{2d})$, the commutator $\frac{i}{\varepsilon}\left[\hat{H}^\varepsilon, \mathrm{op}_\varepsilon(a)\right]$ is uniformly bounded with respect to ε (what we have indirectly obtained during the calculations in this section), so, from (2.2.10), one sees that the family $t \longmapsto \left\langle \mathrm{op}_{\varepsilon_k}(a)\Psi^{\varepsilon_k}, \Psi^{\varepsilon_k}\right\rangle$ is equicontinuous in $[-T,T]$ in addition to being equibounded, which implies the continuity of $[-T,T] \ni t \longmapsto \langle \mu_t, a\rangle_{\mathbb{R}^{2d}}$ by the Ascoli-Arzelà theorem.

This is not true for ν_t in general, as the examples in Theorem 3.4.1 show. In both cases there, we have $\int_{\mathcal{S}^0} \nu_t(d\omega) = 0$ for any $t \neq 0$ and $\int_{\mathcal{S}^0} \nu_0(d\omega) = 1$, so $\nu_t \neq 0$ if and only if $t = 0$, which is a lack of continuity for ν_t in spite of μ_t.

Consequently, it makes no sense to think of ν on a t by t basis unless directly linked to μ, as in Lemma 2.3.7. In particular, observe that there may be violations of the asymmetry condition (3.2.2) for a particular instant t or, more generally, for time sets with null Lebesgue measure. This is not at all a contradiction, since this condition is only valid *in average* in time.

On the other hand, one could use an argument of continuity for μ_t to see, in the one-dimensional case $V(x) = \|x\|$, that a family $(\Psi_t^\varepsilon)_{\varepsilon>0}$ whose initial data concentrate to $\mu_0(x,\xi) = \delta(x)\otimes\delta(\xi)$ will remain concentrating to this same point, $\mu_t = \delta(x)\otimes\delta(\xi)$. In this case, condition (3.2.2) allows a complete description of ν:

$$\nu(t,\omega) = \frac{1}{2}\left(\delta(\omega-1) + \delta(\omega+1)\right)\otimes dt.$$

In Section 11.1, we will work out more deeply some issues related to the measures' time continuity. There, more specifically in Examples 11.1.1 and 11.1.2, we will be in a situation where there is no *a priori* results about the continuity of $t \longmapsto \mu_t$, but, instead, for one of the two-microlocal measures, M. In that context, we will only be able to extrapolate the continuity of the operator-valued measures $t \longmapsto M_t$ to μ_t up to a set of times with null Lebesgue measure. As a consequence, the evolution of μ_t will not be given from a hypothetical μ_0, but rather be linked to the evolution of the microlocal measure M_t starting from its initial datum M_0.

Chapter 5

The classical flow and the regime change

5.1 The concentration of ν

In last section we presented a trivial application of the asymmetry condition (3.2.2). In this section we will apply it to obtain Theorem 3.3.2. Moreover, we will prove Theorems 3.3.3 and 3.3.4. In next section we will give examples of applications of these results.

So, to start with:

Proof of Theorem 3.3.2. Since V_S and $F^t\nabla g$ are continuous functions all over $\mathbb{R}^d$, there exists a neighbourhood Γ of σ such that the inequality

$$\left\|F(x)^t\nabla g(x)\right\|_{\mathcal{L}(N_x\Lambda)} < \|\partial_\rho V_S(x)\|_{N_x\Lambda}$$

holds strictly for every $x \in \Gamma$. Let be $a \in C_0^\infty(\mathbb{R}\times T^*\Gamma)$, and let us test expression (3.2.2) against this function:

$$\left\langle\, \nu(t,\sigma,\zeta,\omega)\,,\, a(t,\sigma,\zeta)\left(\partial_\rho V_S(\sigma) + F(\sigma)^t\nabla g(\sigma)\omega\right) \right\rangle_{\mathbb{R}\times ES\Lambda} = 0.$$

Further, realize that the testing term is always non-zero within the support of a:

$$\begin{aligned}\left\|a(t,\sigma,\zeta)\left(\partial_\rho V_S(\sigma) + F(\sigma)^t\nabla g(\sigma)\omega\right)\right\|_{N_\sigma\Lambda} &\geqslant |a(t,\sigma,\zeta)|\left(\|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda} - \left\|F(\sigma)^t\nabla g(\sigma)\omega\right\|_{N_\sigma\Lambda}\right)\\ &> 0;\end{aligned}$$

as a consequence, since ν is always positive, one must have $\nu = 0$ over the support of a, more precisely, over $ES\Gamma$. □

5.2 The study of the classical flow

Now, in order to study the classical flow in more details, remark that in the transformed coordinates introduced in Section 4.1, the equation of motion for the component of x in Λ, x', reads:

$$\begin{cases}\dot{x}'(t) = D_g(x(t))\xi'(t)\\ \dot{\xi}'(t) = -\partial_{x'}V_S(x(t)) - \|x'(t)\|\partial_{x'}F(x(t)) - F(x(t))\frac{x'(t)}{\|x'(t)\|}.\end{cases}$$

Let us suppose that $(x(t),\xi(t))$ is a trajectory that reaches the phase space singular set Ω on the point $\sigma\in\Lambda$ at a time $t=0$, so we have $x'(0)=0$ and $\xi'(0)=0$. Calculate:

$$x'(t)=t\int_0^1\dot{x}'(st)ds \qquad \text{and} \qquad \dot{x}'(st)=\dot{x}'(0)+t\int_0^s\ddot{x}'(rt)dr,$$

where $\dot{x}'(0)=D_g(x(0))\,\xi'(0)=0$ and

$$\ddot{x}'(t)=\left(\nabla_x D_g(x(t))\,\xi(t)\right)\xi'(t)+D_g(x(t))\dot{\xi}'(t).$$

Then, for $t\neq 0$, we can define a $\theta(t)=\frac{2}{t^2}x'(t)$ that reads:

$$\theta(t)=2\int_0^1\int_0^s\left(\left(\nabla_x D_g(x(rt))\,\xi(rt)\right)\xi'(rt)+D_g(x(rt))\right.$$
$$\left.\left(-\partial_{x'}V_S(x(rt))-\|x'(rt)\|\partial_{x'}F(x(rt))-F(x(rt))\frac{x'(rt)}{\|x'(rt)\|}\right)\right)drds, \tag{5.2.1}$$

where D_g was defined in Remark 4.2.1; for the reader's convenience, recall that

$$D_g(x)=\nabla g\left(\phi^{-1}(x)\right)^t\nabla g\left(\phi^{-1}(x)\right)$$

is an invertible matrix for $x=(0,x'')$.

Also, let be $(t_n)_{n\in\mathbb{N}}$ such that $t_n\longrightarrow 0$. Necessarily the sequence $\frac{x'(t_n)}{\|x'(t_n)\|}$ will have convergent subsequences. If all possible sequences $\frac{x'(t_n)}{\|x'(t_n)\|}$ with $t_n>0$ tending to 0 converge to the same limit $\frac{\theta_0^+}{\|\theta_0^+\|}$, we call it the *positive lateral limit* of the function $\frac{x'(t)}{\|x'(t)\|}$ and denote $\frac{\theta_0^+}{\|\theta_0^+\|}=\lim_{t\to 0^+}\frac{x'(t)}{\|x'(t)\|}$; in the same way, one can talk about *negative lateral limits*. Finally, we define the lateral limits of $\theta(t)=\frac{1}{t^2}x'(t)$ in an analogous manner, when they exist.

Lemma 5.2.1. *Fix a vector $\theta_0\in\mathbb{R}^p$, $\theta_0\neq 0$. If θ_0 is a lateral limit of $\theta(t)$, then $\frac{\theta_0}{\|\theta_0\|}$ is a lateral limit of $\frac{x'(t)}{\|x'(t)\|}$, either both positive, or both negative. Conversely, if $\frac{\theta_0}{\|\theta_0\|}$ is a lateral limit of $\frac{x'(t)}{\|x'(t)\|}$, then there exists $\lambda\geqslant 0$ such that $\lambda\theta_0$ is a lateral limit of $\theta(t)$.*

Besides, θ_0 is a solution to the equation

$$\lambda D_g^{-1}(x(0))\theta_0=-\partial_{x'}V_S(x(0))-F(x(0))\frac{\theta_0}{\|\theta_0\|}; \tag{5.2.2}$$

geometrically, this equation reads (remembering that ∂_ρ is the derivative normal to Λ):

$$\lambda\rho_0=-\partial_\rho V_S(\sigma)-F(\sigma)^t\nabla g(\sigma)\frac{\nabla g(\sigma)\rho_0}{\|\nabla g(\sigma)\rho_0\|}, \tag{5.2.3}$$

where ρ_0 is a lateral limit of the $N_\sigma\Lambda$ vector function $\frac{1}{t^2}\nabla g(x(t))^{-1}g(x(t))$.

Finally, if $\|F(\sigma)^t\nabla g(\sigma)\|_{\mathcal{L}(N_\sigma\Lambda)}<\|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}$ and $\frac{x'(t)}{\|x'(t)\|}$ converges laterally, then any lateral limit $\lambda\theta_0$ of $\theta(t)$ is non-zero and, therefore, satisfies the above equations with $\lambda\neq 0$.

Proof. Observe that $\frac{x'(t)}{\|x'(t)\|} = \frac{\theta(t)}{\|\theta(t)\|}$ for any $t \neq 0$, so if θ_0 is non-zero and a lateral limit of $\theta(t)$, then necessarily $\frac{\theta_0}{\|\theta_0\|}$ is a lateral limit of $\frac{x'(t)}{\|x'(t)\|}$. The converse comes from the definition of $\theta(t)$ in (5.2.1): since at the limit $t \longrightarrow 0$ one has the full limits $\xi'(t) \longrightarrow 0$, $x'(t) \longrightarrow 0$, $V_S(x(t)) \longrightarrow V_S(\sigma)$ and $F(x(t)) \longrightarrow F(\sigma)$, then whenever $\frac{x'(t)}{\|x'(t)\|}$ converges laterally to some limit $\frac{\theta_0}{\|\theta_0\|}$, $\theta(t)$ also converges laterally to a well-defined vector $\tilde{\theta}$. If it is non-zero, by the previous identity $\frac{x'(t)}{\|x'(t)\|} = \frac{\theta(t)}{\|\theta(t)\|}$ one must have $\frac{\tilde{\theta}}{\|\tilde{\theta}\|} = \frac{\theta_0}{\|\theta_0\|}$, so $\tilde{\theta} = \lambda\theta_0$ with $\lambda > 0$; if it is zero, then $\tilde{\theta} = \lambda\theta_0$ for $\lambda = 0$, and we get the lemma's first paragraph either way.

Equation (5.2.2) comes from taking lateral limits in equation (5.2.1) when $\frac{\theta_0}{\|\theta_0\|}$ is a lateral limit of $\frac{x'(t)}{\|x'(t)\|}$ and $\lambda\theta_0$ of $\theta(t)$. Multiplying its both sides by ${}^t\nabla g(\sigma)$, one gets

$$\lambda\nabla g(\sigma)^{-1}\theta_0 = -\partial_\rho V_S(\sigma) - F(\sigma)^t\nabla g(\sigma)\frac{\theta_0}{\|\theta_0\|}. \tag{5.2.4}$$

Two things remain before completing the proof: recognizing equation (5.2.3) from (5.2.4) and, if $\frac{x'(t)}{\|x'(t)\|}$ has lateral limits, proving that any lateral limit $\theta(t)$ is non-zero under the additional hypothesis that

$$\|F(\sigma)^t\nabla g(\sigma)\|_{\mathcal{L}(N_\sigma\Lambda)} < \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda}.$$

The latter is done by remarking that, if $\|F(\sigma)^t\nabla g(\sigma)\| < \|\partial_\rho V_S(\sigma)\|$, surely

$$\lambda\nabla g(\sigma)^{-1}\theta_0 \neq 0$$

by the same arguments we saw in the proof of Theorem 3.3.2), so $\lambda \neq 0$.

Finally, recall that x' is the coordinate of the variable in the normal bundle $N_\sigma\Lambda$; calling it ρ in the original coordinates, we have $x' = \nabla g(\sigma)\rho$, so in (5.2.4) we have just a lateral limit of $\frac{2}{t^2}\rho(t) = \frac{2}{t^2}\nabla g(\sigma)^{-1}x'(t)$: $\theta_0 = \nabla g(\sigma)\rho_0$. $\square$

As we have seen in the lemma above, for any trajectory arriving on Ω within a well-defined direction θ_0, *i.e.*, such that $\lim_{t\to 0^-} \frac{x'(t)}{\|x'(t)\|} = \frac{\theta_0}{\|\theta_0\|}$, if

$$\|F(\sigma)^t\nabla g(\sigma)\|_{\mathcal{L}(N_\sigma\Lambda)} < \|\partial_\rho V_S(\sigma)\|_{N_\sigma\Lambda},$$

then this direction is submitted to satisfy equation (5.2.2) with $\lambda \neq 0$, which implies, in particular, that if this equation has no non-zero roots, then by absurd no trajectory at all can reach Ω.

Regarding the inverse affirmation, Lemma 5.2.1 does not say whether there are actual trajectories approaching Ω in all possible directions satisfying (5.2.2). Below we will verify that indeed any θ_0 satisfying (5.2.2) is realized as an approaching direction by some Hamiltonian trajectory.

Lemma 5.2.2. *If* $\theta_0^+, \theta_0^- \neq 0$ *satisfy* (5.2.2)*, then there exists a unique trajectory* $(x(t), \xi(t))$ *reaching* Ω *at* $t = 0$ *in a point* $\sigma \in \Lambda$ *such that* $\lim_{t\to 0^\pm} \frac{x'(t)}{\|x'(t)\|} = \frac{\theta_0^\pm}{\|\theta_0^\pm\|}$.

Proof. First, let us choose $\theta_0^+ = \theta_0^- = \theta_0$. For x_0 and ξ_0 such that $x_0' = \xi_0' = 0$ and so that x_0 is the coordinate of σ, take $\tau > 0$, $\lambda > 0$ and $0 < \delta < \|\theta_0\|$ sufficiently small so as the set

$$\mathcal{B}^{[-\tau,\tau]} = \Big\{(x,\xi,\vartheta) \in \left(C^0\left([-\tau,\tau]\right)\right)^3 : (x,\xi,\vartheta)(0) = (x_0,\xi_0,\lambda\theta_0) \text{ and } \sup_{t\in[-\tau,\tau]} \left(\|x(t)-x_0\| + \|\xi(t)-\xi_0\| + \|\vartheta(t)-\lambda\theta_0\|\right) \leqslant \delta\Big\}$$

fits in a proper definition of the application $\mathfrak{F} : \mathcal{B}^{[-\tau,\tau]} \longrightarrow \mathcal{B}^{[-\tau,\tau]}$ given by:

$$\mathfrak{F}_x(x,\xi,\vartheta)(t) = x_0 + \int_0^t D(x(s))\,\xi(s)ds,$$

$$\mathfrak{F}_\xi(x,\xi,\vartheta)(t) = \xi_0 + \int_0^t \left(-\nabla V_S(x(s)) - \|x'(s)\|\nabla F(x(s)) - F(x(s))\frac{(\vartheta(s),\mathbf{0}_{\mathbb{R}^{d-p}})}{\|\vartheta(s)\|}\right) ds$$

and last

$$\mathfrak{F}_\vartheta(x,\xi,\vartheta)(t) = 2\lambda \int_0^1 \int_0^s \left((\nabla_x D_g(x(rt))\,\xi(rt))\,\xi'(rt) + D_g(x(rt))\right.$$
$$\left.\left(-\partial_{x'} V_S(x(rt)) - \|x'(rt)\|\partial_{x'} F(x(rt)) - F(x(rt))\frac{\vartheta(rt)}{\|\vartheta(rt)\|}\right)\right) drds.$$

Observe that $\mathcal{B}^{[-\tau,\tau]}$ is a set which is complete with respect to its natural supremum norm employed in its definition. Observe further that, by taking λ and τ as small as necessary, $\mathfrak{F}$ becomes a contraction on $\mathcal{B}^{[-\tau,\tau]}$ equipped with its topology, *i.e.*, there exists $0 < K < 1$ such that

$$\sup_{t\in[-\tau,\tau]} \left(\|\mathfrak{F}_x(x,\xi,\vartheta)(t) - x_0\| + \|\mathfrak{F}_\xi(x,\xi,\vartheta)(t) - \xi_0\| + \|\mathfrak{F}_\vartheta(x,\xi,\vartheta)(t) - \lambda\theta_0\|\right)$$
$$\leqslant K \sup_{t\in[-\tau,\tau]} \left(\|x(t)-x_0\| + \|\xi(t)-\xi_0\| + \|\vartheta(t)-\lambda\theta_0\|\right).$$

Consequently, by Banach's fixed point theorem, there exists a unique triple $(x,\xi,\vartheta) \in \mathcal{B}^{[-\tau,\tau]}$ such that $(x,\xi,\vartheta) = \mathfrak{F}(x,\xi,\vartheta)$; this is equivalent to saying that the system

$$\begin{cases} \dot{x}(t) = D(x(t))\xi(t) \\ \dot{\xi}(t) = -\nabla V_S(x(t)) - \|x'(t)\|\nabla F(x(t)) - F(x(t))\frac{(\vartheta(t),\mathbf{0}_{\mathbb{R}^{d-p}})}{\|\vartheta(t)\|} \\ \frac{d}{dt}\left(\frac{t^2}{2}\vartheta(t)\right) = \lambda\dot{x}'(t) \end{cases}$$

with initial data $(x_0,\xi_0,\lambda\theta_0)$ admits a unique solution, which must be such that $\frac{\vartheta(t)}{\|\vartheta(t)\|} = \frac{x'(t)}{x'(t)}$ $\forall t \neq 0$. Therefore, $(x(t),\xi(t))$ must be a trajectory of our conical problem with the properties listed in the lemma for $\theta_0 = \theta_0^+ = \theta_0^-$.

For $\theta_0^+ \neq \theta_0^-$, define the sets $\mathcal{B}^{[0,\tau]}$ and $\mathcal{B}^{[-\tau,0]}$ and proceed as above in order to show the existence for $\pm t \in [0,\tau]$ of trajectories $(x_\pm(t),\xi_\pm(t))$ such that $\lim_{t\longrightarrow 0^\pm} \frac{x'_\pm(t)}{\|x'_\pm(t)\|} = \frac{\theta_0^\pm}{\|\theta_0^\pm\|}$. Besides, as $\lim_{t\longrightarrow 0^\pm} x_\pm(t) = x_0$ and $\lim_{t\longrightarrow 0^\pm} \xi_\pm(t) = \xi_0$, we can build a continuous path $(x(t),\xi(t))$ by setting $x(t) = x_\pm(t)$ and $\xi(t) = \xi_\pm(t)$ for $\pm t \geqslant 0$, and this new trajectory will be Hamiltonian and the unique one to meet the properties stated in the lemma. □

Bringing together Lemmata 5.2.1 and 5.2.2, one proves Theorem 3.3.3. In order to obtain Theorem 3.3.4, we observe the following facts:

1. The hypothesis $\|F(\sigma)^t\nabla g(\sigma)\| < \|\partial_\rho V_S(\sigma)\|$ played no role in the demonstration of Lemma 5.2.2, nor in the proof of Lemma 5.2.1, where we could have $\theta_0 \neq 0$ and $\tilde{\theta} = 0$. In any case, if some trajectory is to arrive onto Ω in σ with some well-defined direction, then either (3.3.2) or (3.3.3) must be satisfied.

2. If θ_0 is a "zero root" of (5.2.2) (otherwise said, $\tilde{\theta} = \lambda\theta_0$ with $\lambda = 0$), then we will see in Example 5.3.3 that it may happen that no trajectory following the direction θ_0 ever touches Ω in σ. On the other hand, in Example 5.3.4 we will see a case where there is a trajectory approaching the singularity, but only asymptotically.

The proof of Theorem 3.3.4 will be complete after showing that any such trajectories only reach Ω after an infinite time. Letting be $(x(t), \xi(t))$ a trajectory that is not on Ω at $t = 0$, define

$$\Upsilon = \{t \in \mathbb{R} : \forall s \in [0, t], (x(s), \xi(s)) \notin \Omega\}$$

and $\Gamma = \{(x(t), \xi(t)) : t \in \Upsilon\}$.

Lemma 5.2.3. *If $\theta_0 \neq 0$ obeys to (5.2.2) with $\lambda = 0$ and we suppose that there is a trajectory $(x(t), \xi(t))$ such that $(x(0), \xi(0)) \notin \Omega$, that for any $\varepsilon > 0$ there is $t_\varepsilon > 0$ for which $\|(x'(t_\varepsilon), \xi'(t_\varepsilon))\| < \varepsilon$ and such that $\lim_{\varepsilon\to 0} \frac{1}{\|x'(t_\varepsilon)\|} x'(t_\varepsilon) = \frac{\theta_0}{\|\theta_0\|}$, then $\sup \Upsilon = \infty$.*

Proof. From the hypotheses $\theta_0 \neq 0$ and $\lambda = 0$ in (5.2.2), it follows that $\lim_{\varepsilon\to 0} \partial_{x'} V(x(t_\varepsilon)) = 0$; as a consequence, it becomes possible to find a smooth extension $\tilde{V}$ of V outside the closure of Γ such that $\partial_{x'}\tilde{V}(\sigma) = 0$ and that $\tilde{V}(x(t)) = V(x(t))$ for any $t \in \Upsilon$.

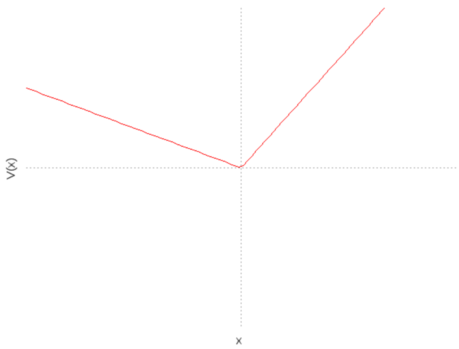
Then $(x'(t), \xi'(t))$ is at the same time a Hamiltonian trajectory of a conical potential and of a standard problem with smooth potential, for which case it is widely known that no trajectory can arrive at an extremum of $\tilde{V}$ with null speed ξ' within a finite time (since this would break the unicity of the constant solution $(x'(t), \xi'(t)) = (0, 0)$). □

5.3 Examples of classification for the semiclassical transport

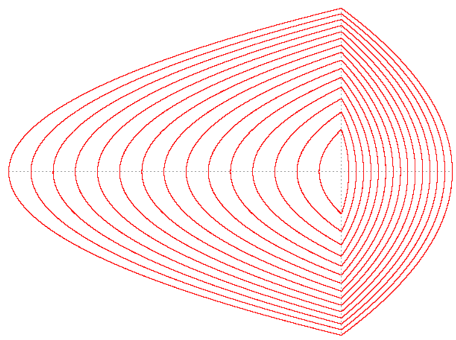
In this section we will give examples of how Theorems 3.3.2, 3.3.3 and 3.3.4 can be used in order to classify the trajectories that arrive on a conical singularity and, sometimes, to completely describe the transport phenomenon to which the semiclassical measures are submitted. In particular, Examples 5.3.3 and 5.3.4 are part of the reasoning that led to obtaining the second assertive in Theorem 3.3.4.

To begin with, let us consider $d = 1$ and $g(x) = x$, so $\nabla g(x) = 1$.

Example 5.3.1 ($|\nabla V_S(\sigma)| < |F(\sigma)|$ with no roots). Take $V_S(x) = \frac{1}{2}x$ and $F(x) = 1$.



$V(x) = \frac{1}{2}x + |x|$



Φ, example 5.3.1

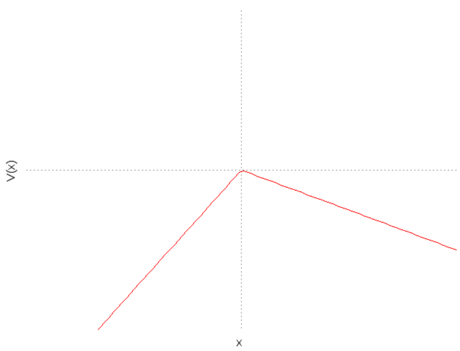
Then (3.3.2) admits no non-zero solutions, which is consistent with the fact that the classical flow Φ presents no trajectories hitting the singularity.

In this case, the asymmetry condition (3.2.2) gives that

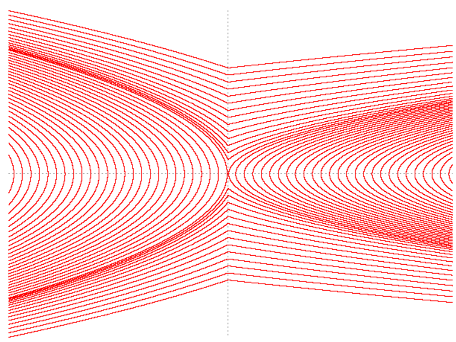
$$\nu(t,\omega) = p\left(\frac{1}{4}\delta(\omega-1) + \frac{3}{4}\delta(\omega+1)\right) \otimes dt,$$

with $0 \leqslant p \leqslant 1$ the total mass over the singularity and does not depend on t. The semiclassical transport here is thus completely solvable starting from some initial measure.

Example 5.3.2 ($|\nabla V_S(\sigma)| < |F(\sigma)|$ with non-zero roots). Consider $V_S(x) = \frac{1}{2}x$ and take $F(x) = -1$.



$V(x) = \frac{1}{2}x - |x|$



Φ, example 5.3.2

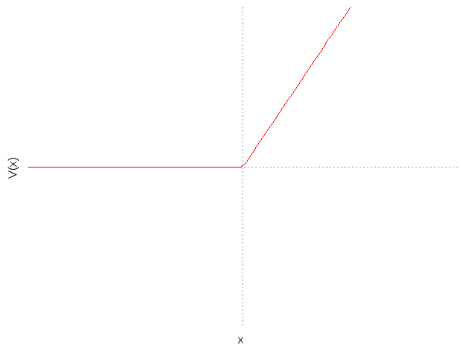
Then (3.3.2) admits two solutions: $\rho_0 = \frac{1}{2}$ and $\rho_0 = -\frac{3}{2}$, which is consistent with the fact that the classical flow Φ does present trajectories hitting the singularity from both directions $x > 0$ and $x < 0$.

In this case, we will have

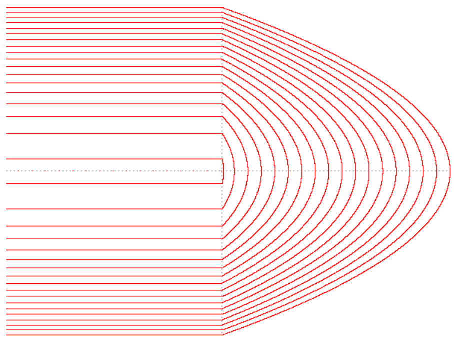
$$\nu(t,\omega) = p(t)\left(\frac{3}{4}\delta(\omega-1) + \frac{1}{4}\delta(\omega+1)\right) \otimes dt,$$

with $0 \leqslant p(t) \leqslant 1$ the total mass over the singularity, which may vary with t.

Example 5.3.3 ($|\nabla V_S(\sigma)| = |F(\sigma)|$, with zero-roots without trajectories). Take $V_S(x) = x$ and $F(x) = 1$.



$V(x) = x + |x|$



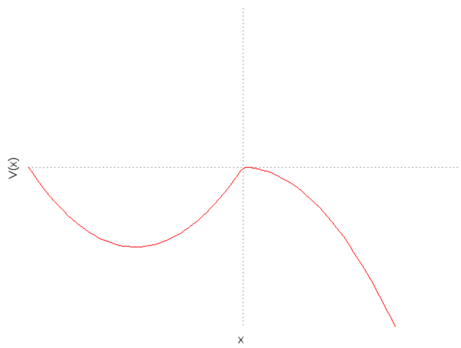
Φ, example 5.3.3

Then equation (3.3.2) has no non-zero roots, but equation (3.3.3) admits any solution $\rho_0 < 0$. In this case, there are no trajectories hitting the singularity from $x < 0$. The semiclassical measure in sphere will be

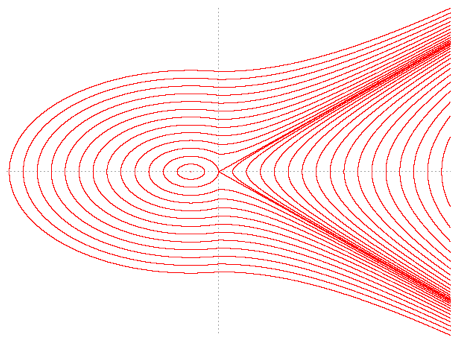
$$\nu(t,\omega) = p\,\delta(\omega+1) \otimes dt,$$

where the total mass over the singularity $0 \leqslant p \leqslant 1$ is constant. Again, this is a completely solvable case.

Example 5.3.4 ($|\nabla V_S(\sigma)| = |F(\sigma)|$ with non-zero and zero roots with trajectories). Pick up $V_S(x) = x$ and $F(x) = -(1+x)$.



$V(x) = x - (1+x)|x|$



Φ, example 5.3.4

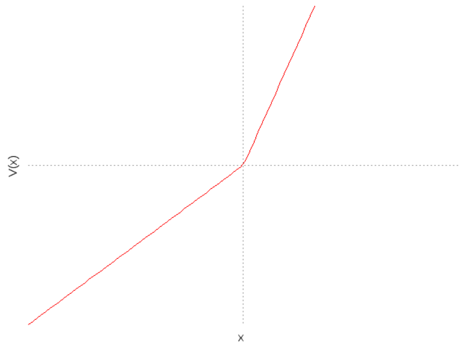
Then equation (3.3.2) admits one solution: $\rho_0 = -2$, and equation (3.3.3) also admits solutions: any $\rho_0 > 0$. This is consistent with the fact that the classical flow Φ presents a trajectory hitting the singularity from the direction $x < 0$, and in this case also from the direction $x > 0$. However, the trajectory from the positive side takes an infinitely long time to get close to the singularity.

One has:

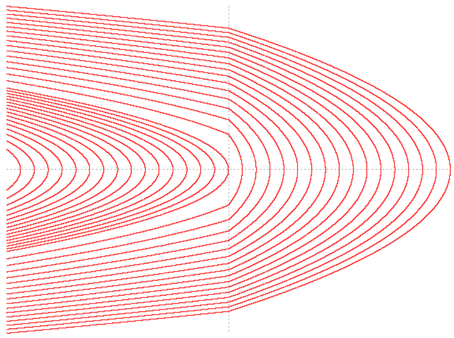
$$\nu(t, \omega) = p(t)\, \delta(\omega + 1) \otimes dt,$$

the total mass on the singularity possibly changing with time.

Example 5.3.5 ($|\nabla V_S(\sigma)| > |F(\sigma)|$ with a unique trajectory). Take $V_S(x) = 2x$ and choose $F(x) = 1$.



$V(x) = 2x + |x|$



Φ, example 5.3.5

Then equation(3.3.2) admits a unique solution: $\rho_0 = -3$, which is consistent with the fact that the classical flow Φ only presents a trajectory hitting the singularity from the direction $x < 0$.

In this case, since $|\nabla V_S(0)| > |F(0)|$, we will have $\nu = 0$, so the semiclassical measure will necessarily follow the exterior flow with the singularity being part of the parabola passing through the origin from $x < 0$. The problem is hence completely solvable, even though there are trajectories leading to the singular set.

Now let be $p = d = 3$ and denote $x = (x_1, x_2, x_3)$.

Example 5.3.6 ($\|\nabla V_S(\sigma)\| > \|F(\sigma)^t \nabla g(\sigma)\|$ with no trajectories). Choose an exterior potential $V_S(x) = -2x_1$, $F(x) = -1$ and $g(x) = \left(\frac{1}{2}x_1, x_2, x_3\right)$. Then

$$\|\nabla V_S(0)\| = 2 > 1 = \|F(0)^t \nabla g(0)\|$$

and no ρ_0 satisfies equation (3.3.2). As a conclusion, no trajectory in this case can hit the singularity at $x = 0$.

Example 5.3.7 ($\|\nabla V_S(\sigma)\| > \|F(\sigma)^t \nabla g(\sigma)\|$ with many trajectories). Last, we will take the same $V_S(x) = -2x_1$, $F(x) = -1$, but $g(x) = \left(\frac{1}{3}x_1, x_2, x_3\right)$. Then

$$\|\nabla V_S(0)\| = 2 > 1 = \|F(0)^t \nabla g(0)\|,$$

but now equation (3.3.2) admits any solution $\rho_0 = \left(\frac{9}{4}, \rho_2, \rho_3\right)$ with $\rho_2^2 + \rho_3^2 = \frac{7}{16}$. This is a case where the exterior force polarizes the flow in its direction, but leaves it free to spin around a circle of radius $\frac{\sqrt{7}}{4}$ in the orthogonal plane.

Chapter 6

Approximative solutions

6.1 The wave packets

For a $C^2(\mathbb{R}^d)$ potential V and one of its Hamiltonian trajectories $(x(t), \xi(t))$, we define the wave packet with initial profile $v_0 \in L^2(\mathbb{R}^d)$ following $(x(t), \xi(t))$ as

$$\varphi_t^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{d}{4}}} v_t\left(\frac{x - x(t)}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}[\xi(t)\cdot(x - x(t)) + S(t)]}, \tag{6.1.1}$$

where S is the classical action $S(t) = \int_0^t \left(\frac{1}{2}\xi^2(s) - V(x(s))\right) ds$ and v satisfies the ε-independent differential system

$$\begin{cases} i\partial_t v_t(y) = -\frac{1}{2}\Delta v_t(y) + \left(\frac{1}{2}\nabla^2 V(x(t))\, y \cdot y\right) v_t(y) \\ v_{t=0}(y) = v_0(y). \end{cases} \tag{6.1.2}$$

Lemma 6.1.1. *Any semiclassical measure associated to the family $(\varphi^\varepsilon)_{\varepsilon>0}$ is*

$$\mu_t(x,\xi) = \|v_0\|^2_{L^2(\mathbb{R}^d)}\, \delta(x - x(t)) \otimes \delta(\xi - \xi(t)).$$

Proof. A straightforward calculation. Writing down $\langle \mathrm{op}_\varepsilon(a)\, \varphi_t^\varepsilon, \varphi_t^\varepsilon\rangle$ for some $a \in C_0^\infty(\mathbb{R}^{2d})$, performing some variable changes and a Taylor expansion:

$$\begin{aligned} \langle \mathrm{op}_\varepsilon(a)\, \varphi_t^\varepsilon, \varphi_t^\varepsilon\rangle &= \frac{1}{(2\pi\sqrt{\varepsilon})^d}\int_{\mathbb{R}^{3d}} e^{i\xi\cdot(x-y)} a\left(\frac{x+y}{2} + x(t), \varepsilon\xi + \xi(t)\right) v_t\left(\frac{y}{\sqrt{\varepsilon}}\right)\overline{v_t\left(\frac{x}{\sqrt{\varepsilon}}\right)} d\xi dy dx \\ &= \frac{1}{(2\pi\sqrt{\varepsilon})^d}\int_{\mathbb{R}^{3d}} e^{i\xi\cdot(x-y)} a\left(\frac{x+y}{2} + x(t), \xi(t)\right) v_t\left(\frac{y}{\sqrt{\varepsilon}}\right)\overline{v_t\left(\frac{x}{\sqrt{\varepsilon}}\right)} d\xi dy dx + R^\varepsilon, \end{aligned}$$

then integrating in ξ, which gives a Dirac delta, then in y and changing variables once more:

$$\langle \mathrm{op}_\varepsilon(a)\, \varphi_t^\varepsilon, \varphi_t^\varepsilon\rangle = \int_{\mathbb{R}^d} a\left(\sqrt{\varepsilon}x + x(t), \xi(t)\right) |v_t(x)|^2\, dx + R^\varepsilon.$$

The result comes from letting ε go to 0, where the dominated convergence theorem intervenes inside the integral, and from evaluating the remainder:

$$\begin{aligned} R^\varepsilon &= \frac{\varepsilon}{(2\pi\sqrt{\varepsilon})^d}\int_{\mathbb{R}^{3d}}\int_0^1 e^{i\xi\cdot(x-y)}\xi\cdot\partial_\xi a\left(\frac{x+y}{2} + x(t), \varepsilon s\xi + \xi(t)\right) v_t\left(\frac{y}{\sqrt{\varepsilon}}\right)\overline{v_t\left(\frac{x}{\sqrt{\varepsilon}}\right)} ds d\xi dy dx \\ &= \frac{i\varepsilon}{(2\pi\sqrt{\varepsilon})^d}\int_{\mathbb{R}^{3d}}\int_0^1 e^{i\xi\cdot(x-y)}\, \mathrm{tr}\left(\partial_x\partial_\xi a\left(\frac{x+y}{2} + x(t), \varepsilon s\xi + \xi(t)\right)\right) v_t\left(\frac{y}{\sqrt{\varepsilon}}\right)\overline{v_t\left(\frac{x}{\sqrt{\varepsilon}}\right)} ds d\xi dy dx \\ &\sim \mathcal{O}(\varepsilon), \end{aligned}$$

which completes the proof. ∎

Another virtue of the wave packets is that they provide approximative solutions to the Schrödinger equation with convenient initial data, as stated in:

Proposition 6.1.2. *For fixed initial* $(x_0, \xi_0) \in \mathbb{R}^{2d}$*, consider a Hamiltonian trajectory* $(x(t), \xi(t))$ *for a potential* V *not necessarily smooth everywhere over the space trajectory. Let be* $]0, \tau[\subset \mathbb{R}$ *and* $\Upsilon = \left\{x \in \mathbb{R}^d : x = x(t) \text{ for } t \in \,]\, 0, \tau[\right\}$*. If* $\nabla^2 V$ *exists and is Lebesgue integrable in* Υ*, and if* Ψ^ε *is the solution of the Schrödinger equation with potential* V *and initial data* $\Psi_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} v_0\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}\xi_0 \cdot (x-x_0)}$*, then letting be* φ^ε *the wave packet initially centred in* (x_0, ξ_0) *with profile* v_0*, we have*

$$\|\Psi_\tau^\varepsilon - \varphi_\tau^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant \int_{]0,\tau[} \left\|\frac{1}{\varepsilon} R_s^\varepsilon v_s\right\|_{L^2(\mathbb{R}^d)} ds,$$

where

$$R_t^\varepsilon(y) = V\left(x(t) + \sqrt{\varepsilon} y\right) - V(x(t)) - \sqrt{\varepsilon} \nabla V(x(t))\, y - \frac{\varepsilon}{2} \nabla^2 V(x(t))\, y \cdot y. \tag{6.1.3}$$

Proof. After a direct calculation, one obtains the following differential system for φ^ε:

$$\begin{cases} i\varepsilon \partial_t \varphi_t^\varepsilon(x) = \hat{H}^\varepsilon \varphi_t^\varepsilon(x) - R_t^\varepsilon\left(\frac{x-x(t)}{\sqrt{\varepsilon}}\right) \varphi_t^\varepsilon(x) \\ \varphi_{t=0}^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{d}{4}}} v_0\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}\xi_0 \cdot (x-x_0)}, \end{cases} \tag{6.1.4}$$

where H^ε is the Hamiltonian operator (3.1.3) with V as stated, R^ε is explicitly given by equation (6.1.3). Now, we compare Ψ^ε and φ^ε by evaluating

$$\frac{d}{dt} \|\Psi_t^\varepsilon - \varphi_t^\varepsilon\|_{L^2(\mathbb{R}^d)}^2 = 2 \operatorname{Re} \langle \Psi_t^\varepsilon - \varphi_t^\varepsilon, \partial_t(\Psi_t^\varepsilon - \varphi_t^\varepsilon)\rangle_{L^2(\mathbb{R}^d)},$$

which gives, in view of the equations for Ψ^ε, φ^ε and the self-adjointness of H^ε,

$$\frac{d}{dt} \|\Psi_t^\varepsilon - \varphi_t^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant \left\|\frac{1}{\varepsilon} R_t^\varepsilon v_t\right\|_{L^2(\mathbb{R}^d)},$$

thus, for any $\alpha, \beta \in \,]0, \tau[$, we have

$$\left\|\Psi_\beta^\varepsilon - \varphi_\beta^\varepsilon\right\|_{L^2(\mathbb{R}^d)} - \|\Psi_\alpha^\varepsilon - \varphi_\alpha^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant \left|\int_\alpha^\beta \left\|\frac{1}{\varepsilon} R_s^\varepsilon v_s\right\|_{L^2(\mathbb{R}^d)} ds\right|.$$

Naturally, the function $t \longmapsto \|\Psi_t^\varepsilon - \varphi_t^\varepsilon\|_{L^2(\mathbb{R}^d)}$ is continuous and, at $t = 0$, $\Psi_0^\varepsilon(x) = \varphi_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{d}{4}}} v_0\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}\xi_0 \cdot x_0}$. Hence, by choosing sequences α_n and β_n in $]0, \tau[$ such that $\alpha_n \longrightarrow 0$ and $\beta_n \longrightarrow \tau$, the proposition follows. ☐

Corollary 6.1.3. *Call* μ *the semiclassical measure linked to the exact family of solutions* $(\Psi^\varepsilon)_{\varepsilon>0}$ *with initial data as in the theorem above. If* $\nabla^3 V$ *exists and is Lebesgue integrable, then*

$$\|\Psi_t^\varepsilon - \varphi_t^\varepsilon\|_{L^2(\mathbb{R}^d)} \lesssim |t|\sqrt{\varepsilon}$$

and, consequently, given $T > 0$*, for any* $t \in [-T, T]$*,*

$$\mu_t(x, \xi) = \delta(x - x(t)) \otimes \delta(\xi - \xi(t)).$$

Proof. V being at least of class $C^3(\mathbb{R}^d)$, one can verify from a Taylor formula that

$$R^\varepsilon(y,t) = \frac{\varepsilon\sqrt{\varepsilon}}{2}\int_0^1 \nabla^3 V\left(x\left(t\right)+s\sqrt{\varepsilon}y\right)\left(1-s\right)^2 ds,$$

and, moreover, that R^ε introduces in the Schrödinger equation a $L^2(\mathbb{R}^d)$ error of order $\mathcal{O}\left(\varepsilon\sqrt{\varepsilon}\right)$. Thus, from Proposition 6.1.2, it is clear that $\Psi_t^\varepsilon = \varphi_t^\varepsilon + \mathcal{O}\left(|t|\sqrt{\varepsilon}\right)$ in $L^2(\mathbb{R}^d)$; for any $t \in [-T,T]$, this gives, when $\varepsilon \longrightarrow 0$, that the Wigner measure of Ψ^ε shall coincide with that of the wave packets. The conclusion comes from Lemma 6.1.1. □

Remark 6.1.4. Actually, the approximation in the corollary remains good for t smaller than the Ehrenfest time $t_E = \ln\frac{1}{\varepsilon}$, as $\sqrt{\varepsilon}\ln\frac{1}{\varepsilon} \longrightarrow 0$ when $\varepsilon \longrightarrow 0$; more details in [34]. Estimates beyond the Ehrenfest time are given in [101].

Observe that even if V is not as regular as we required, we can still write R^ε as in (6.1.3) for any t such that $\nabla V\left(x\left(t\right)\right)$ and $\nabla^2 V\left(x\left(t\right)\right)$ make sense, although in this case it is not clear which is the order of the approximation the wave packet furnishes, nor even whether it is negligible in the semiclassical limit.

Finally, observe that it is also possible to write the actual solution Ψ^ε with initial state $\Psi_0^\varepsilon = \frac{1}{\varepsilon^{\frac{d}{4}}}v_0\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right)e^{\frac{i}{\varepsilon}\xi_0\cdot(x-x_0)}$ under the wave packet form: one defines a u^ε such that

$$\Psi^\varepsilon\left(x,t\right) = \frac{1}{\varepsilon^{\frac{d}{4}}}u^\varepsilon\left(\frac{x-x\left(t\right)}{\sqrt{\varepsilon}},t\right)e^{\frac{i}{\varepsilon}\left[\xi(t)\cdot(x-x(t))+S(t)\right]}, \tag{6.1.5}$$

which consequently obeys to

$$\begin{cases} i\partial_t u^\varepsilon\left(y,t\right) = -\frac{1}{2}\Delta u^\varepsilon\left(y,t\right) + \left(\frac{1}{2}\nabla^2 V\left(x\left(t\right)\right)y\cdot y\right)u^\varepsilon\left(y,t\right) + \frac{1}{\varepsilon}R^\varepsilon\left(y,t\right)u^\varepsilon\left(y,t\right) \\ u^\varepsilon\left(y,0\right) = v_0(y), \end{cases} \tag{6.1.6}$$

which is nothing else than the exact Schrödinger equation written in a different form.

6.2 Approaching solutions with wave packets

In the Introduction we pointed out that the non-uniqueness of the classical flow for the present case only plays a relevant role when the initial data concentrate to a point belonging to a trajectory that leads to the singularity. The behaviour of the measure will depend on the concentration rate and oscillations of the quantum states Ψ^ε as well as on other characteristics of this family over the crossings, such as the region where these states are supported.

Below, we will prove some results that altogether are slightly more general than Theorem 3.4.1. We will present concrete cases of solutions to the Schrödinger equation with the conical potential $V(x) = -|x|$, $x \in \mathbb{R}$, that concentrate to a branch of one of the parabolæ leading to the singularity in Figure 3.1.1(b), and thereafter either swap to the other parabola (Section 6.2.2, Proposition 6.2.4) or keep on the same one (Sections 6.2.1, Proposition 6.2.1).

These examples refute any possibility of a classical selection principle allowing one to predict the evolution of a particle (*i.e.*, a Wigner measure concentrated to a single point) after it touches the singularity, since they show two particles subjected to the same potential and following the same path for any $t < 0$, but then going each to a different side for $t > 0$.

6.2.1 Measures rebounding at the singularity

Let us consider the trajectories

$$\begin{cases} \xi_\pm(t) = \pm t \\ x_\pm(t) = \pm\frac{t^2}{2} \end{cases} \quad \text{for } t \in \mathbb{R}. \tag{6.2.1}$$

In this section we will prove:

Proposition 6.2.1. *Let be Ψ^ε the solution to the Schrödinger equation* (3.1.2) *with $V(x) = -|x|$ in $\mathbb{R}$ with initial datum*

$$\Psi_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} a\left(\frac{x}{\sqrt{\varepsilon}}\right),$$

with $a \in C_0^\infty(\mathbb{R})$.

For any $t \in \mathbb{R}$ the semiclassical measure associated to the family $(\Psi^\varepsilon)_{\varepsilon>0}$ is given by

$$\mu_t(x,\xi) = p^+\,\delta(x - x_+(t)) \otimes \delta(\xi - \xi_+(t)) + p^-\,\delta(x - x_-(t)) \otimes \delta(\xi - \xi_-(t)),$$

where the weights $p^\pm$ are given by

$$p^\pm = \pm\int_0^{\pm\infty} |a(x)|^2\,dx.$$

Proof. Given an arbitrary $\delta > 0$, let us cut the evolved state Ψ_t^ε into three parts,

$$\Psi_t^\varepsilon(x) = \Psi_{+,t}^{\varepsilon,\delta}(x) + \Psi_{\bullet,t}^{\varepsilon,\delta}(x) + \Psi_{-,t}^{\varepsilon,\delta}(x),$$

where $\Psi_+^{\varepsilon,\delta}$, $\Psi_\bullet^{\varepsilon,\delta}$ and $\Psi_-^{\varepsilon,\delta}$ solve the Schrödinger equation with initial data

$$\begin{array}{rclcl} \Psi_{+,0}^{\varepsilon,\delta}(x) &=& \frac{1}{\varepsilon^{\frac14}} a\left(\frac{x}{\sqrt{\varepsilon}}\right)\chi_+^\delta\left(\frac{x}{\sqrt{\varepsilon}}\right) & & \operatorname{supp}\chi_+^\delta \subset \{x\in\mathbb{R} : x \geqslant \delta\} \\ \Psi_{\bullet,0}^{\varepsilon,\delta}(x) &=& \frac{1}{\varepsilon^{\frac14}} a\left(\frac{x}{\sqrt{\varepsilon}}\right)\chi_\bullet^\delta\left(\frac{x}{\sqrt{\varepsilon}}\right) & \text{with} & \operatorname{supp}\chi_\bullet^\delta \subset \{x\in\mathbb{R} : -2\delta \leqslant x \leqslant 2\delta\} \\ \Psi_{-,0}^{\varepsilon,\delta}(x) &=& \frac{1}{\varepsilon^{\frac14}} a\left(\frac{x}{\sqrt{\varepsilon}}\right)\chi_-^\delta\left(\frac{x}{\sqrt{\varepsilon}}\right) & & \operatorname{supp}\chi_-^\delta \subset \{x\in\mathbb{R} : x \leqslant -\delta\} \end{array}$$

chosen in such a way that $\chi_+^\delta + \chi_\bullet^\delta + \chi_-^\delta = 1$, all these three functions smooth and taking values in $[0,1]$.

The middle term's semiclassical measure has total mass of order $\delta \max_{x\in\mathbb{R}} |a(x)|^2$; as a consequence, the full Wigner measure of Ψ^ε will be, for any $\delta > 0$:

$$\mu = \mu^{\delta,+} + \mu^{\delta,-} + \gamma^\delta + \mathcal{O}(\delta), \tag{6.2.2}$$

where $\mu^{\delta,\pm}$ are the measures associated to $\Psi_\pm^{\varepsilon,\delta}$, $\mathcal{O}(\delta)$ is a measure with total mass of order δ issued from the middle term and its interferences with the other terms, and γ^δ is the interference measure between $\Psi_-^{\varepsilon,\delta}$ and $\Psi_+^{\varepsilon,\delta}$, which satisfies, for any strictly positive test function $b \in S^\infty(\mathbb{R}\times\mathbb{R}^2)$, the estimate

$$\left|\left\langle \gamma^\delta , b \right\rangle\right| \leqslant \sqrt{\langle \mu^{\delta,+} , b\rangle \langle \mu^{\delta,-} , b\rangle}, \tag{6.2.3}$$

as widely known in semiclassical calculus[1]. Remark that γ^{δ} is not necessarily positive.

For the study of $\mu^{\delta,\pm}$, let us introduce $\varphi_{\pm}^{\varepsilon,\delta}$, the wave packets defined in (6.1.1) for $t \in \mathbb{R}$, having profiles $v^{\delta,\pm}$ that obey to

$$(6.2.4) \qquad \begin{cases} i\partial_t v_t^{\delta,\pm}(y) = -\frac{1}{2}\Delta v_t^{\delta,\pm}(y) \\ v_0^{\delta,\pm}(y) = a\,(y)\,\chi_{\pm}^{\delta}\,(y)\,, \end{cases}$$

which is nothing more than the profile equation (6.1.2) *with the smooth potentials* $\tilde{V}^{\pm}(x) = \mp x$ (which admit the trajectories (6.2.1)).

Lemma 6.2.2. *For any* $\delta > 0$*,*

$$\lim_{\varepsilon \longrightarrow 0} \left\| \Psi_{\pm}^{\varepsilon,\delta} - \varphi_{\pm}^{\varepsilon,\delta} \right\|_{L^{\infty}([-T,T],L^2(\mathbb{R}))} = 0.$$

(The proof is postponed.)

So, the Wigner measures for the components $\Psi_{\pm}^{\varepsilon,\delta}$ are the same as those for $\varphi_{\pm}^{\varepsilon,\delta}$, which one computes explicitly:

$$\mu_t^{\delta,\pm}\,(x,\xi) = \pm\delta\,(x - x_{\pm}\,(t)) \otimes \delta\,(\xi - \xi_{\pm}\,(t)) \int_0^{\pm\infty} \left| a\,(y)\ \chi_{\pm}^{\delta}\,(y) \right|^2 dy;$$

observe that Equation (6.2.3) implies that γ^{δ} is supported on the intersection of the supports of $\mu^{\delta,+}$ and $\mu^{\delta,-}$, but from last formula this intersection turns out to be different from the empty set only for $t = 0$, or, more rigorously, it is contained within $\{t = 0\} \times \mathbb{R}^{2d}$. It happens that γ^{δ} is absolutely continuous with respect to $\mu^{\delta,\pm}$, and these are absolutely continuous with respect to the Lebesgue measure dt, as we saw in Section **??**. As a conclusion, $\gamma^{\delta} = 0$.

Finally, as δ is arbitrary, we take the limit $\delta \longrightarrow 0$ and it follows from (6.2.2) that $\mu = \mu^+ + \mu^-$, where:

$$\mu^{\pm}\,(t,x,\xi) = p^{\pm}\,\delta\,(x - x_{\pm}\,(t)) \otimes \delta\,(\xi - \xi_{\pm}\,(t))\,,$$

as we had in the proposition's statement. □

Proof of Lemma 6.2.2. To begin with, since for $t \neq 0$ we have $\nabla^j V(x_{\pm}(t)) = \nabla^j \tilde{V}^{\pm}(x_{\pm}(t))$ for any $j \in \{0,1,2\}$, $\varphi_{\pm}^{\varepsilon,\delta}$ obeys to (6.1.4) with an error $\frac{1}{\varepsilon}R^{\varepsilon,\pm}$ defined according to (6.1.3);

---

[1]As a short justification of this estimate, define $a = \sqrt{b}$, which will also be a smooth function (since b is strictly positive), and this will give $\mathrm{op}_{\varepsilon}(b) = \mathrm{op}_{\varepsilon}(a)^2 + \mathcal{O}(\varepsilon)$ in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$. Now calculate:

$$\begin{aligned} |\langle \mathrm{op}_{\varepsilon}(b)\Psi_+^{\varepsilon}\,,\Psi_-^{\varepsilon}\rangle| &= \left|\left\langle \mathrm{op}_{\varepsilon}(a)^2\Psi_+^{\varepsilon}\,,\Psi_-^{\varepsilon}\right\rangle + \mathcal{O}(\varepsilon)\right| \\ &= |\langle \mathrm{op}_{\varepsilon}(a)\Psi_+^{\varepsilon}\,,\mathrm{op}_{\varepsilon}(a)\Psi_-^{\varepsilon}\rangle + \mathcal{O}(\varepsilon)| \\ &\leqslant \|\mathrm{op}_{\varepsilon}(a)\Psi_+^{\varepsilon}\|\,\|\mathrm{op}_{\varepsilon}(a)\Psi_-^{\varepsilon}\| + \mathcal{O}(\varepsilon) \\ &= \sqrt{\left\langle \mathrm{op}_{\varepsilon}(a)\Psi_+^{\varepsilon}\,,\mathrm{op}_{\varepsilon}(a)\Psi_+^{\varepsilon}\right\rangle\left\langle \mathrm{op}_{\varepsilon}(a)\Psi_-^{\varepsilon}\,,\mathrm{op}_{\varepsilon}(a)\Psi_-^{\varepsilon}\right\rangle} + \mathcal{O}(\varepsilon) \\ &= \sqrt{\left\langle \mathrm{op}_{\varepsilon}(b)\Psi_+^{\varepsilon}\,,\Psi_+^{\varepsilon}\right\rangle\left\langle \mathrm{op}_{\varepsilon}(b)\Psi_-^{\varepsilon}\,,\Psi_-^{\varepsilon}\right\rangle} + \mathcal{O}(\varepsilon); \end{aligned}$$

the result comes in the limit where ε goes to 0.

let us calculate it for $t \neq 0$:

$$\begin{aligned}\frac{1}{\varepsilon} R_t^{\varepsilon,\pm}(y) &= \frac{1}{\varepsilon}\left(-\left|\pm\frac{t^2}{2}+\sqrt{\varepsilon}y\right| + \frac{t^2}{2} \pm \sqrt{\varepsilon}y\right) \\ &= -\frac{2y}{\sqrt{\varepsilon}}\left(\frac{\pm\frac{t^2}{2}+\sqrt{\varepsilon}y}{\left|\pm\frac{t^2}{2}+\sqrt{\varepsilon}y\right|+\frac{t^2}{2}}\right)\mathbb{1}_{\left\{\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}}\right\}},\end{aligned}$$

which gives

$$\left|\frac{1}{\varepsilon} R_t^{\varepsilon,\pm}(y,t)\right| \leqslant 2\frac{|y|}{\sqrt{\varepsilon}}\mathbb{1}_{\left\{\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}}\right\}}. \tag{6.2.5}$$

Additionally, one can solve equation (6.2.4) for the profile $v^{\delta,\pm}$ of $\varphi_{\pm}^{\epsilon,\delta}$ explicitly; writing down its solution,

$$v_t^{\delta,\pm}(y) = e^{\frac{i}{2}t\Delta}\left(a(y)\,\chi_{\pm}^{\delta}(y)\right),$$

it remains clear that $v^{\delta,\pm}$ admits a finite development like

$$v_t^{\delta,\pm}(y) = \left(1+\frac{i}{2}t\Delta\right)\left(a(y)\,\chi_{\pm}^{\delta}(y)\right) + t^2\underbrace{\int_0^1 (1-s)\,\partial_t^2 v_{st}^{\delta,\pm}(y)\,ds}_{\tilde{v}_t^{\delta,\pm}(y)}, \tag{6.2.6}$$

where the first term in the right-hand side has support on $\pm y > 0$.

Remark 6.2.3. From (6.2.4) and the fact that its initial datum is $C_0^{\infty}(\mathbb{R})$, it follows that, for any $T > 0$ and $j, k \in \mathbb{N}$, one has $y^j \partial_t^k v^{\delta,\pm} \in L^{\infty}\left([-T,T], L^2(\mathbb{R})\right)$, which natually implies that $y^j \partial_t^k \tilde{v}^{\delta,\pm} \in L^{\infty}\left([-T,T], L^2(\mathbb{R})\right)$.

Therefore, from expressions (6.2.5) and (6.2.6):

$$\begin{aligned}\left\|\frac{1}{\varepsilon} R_t^{\varepsilon,\pm}\, v_t^{\delta,\pm}\right\|_{L^2(\mathbb{R})} &\leqslant \frac{2}{\sqrt{\varepsilon}}\left\|y\, v_t^{\delta,\pm}(y)\,\mathbb{1}_{\left\{\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}}\right\}}\right\|_{L^2(\mathbb{R})} \\ &= \frac{2t^2}{\sqrt{\varepsilon}}\left\|y\, \tilde{v}_t^{\delta,\pm}(y)\,\mathbb{1}_{\left\{\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}}\right\}}\right\|_{L^2(\mathbb{R})},\end{aligned}$$

which results in

$$\sup_{\pm t \in [0,T]}\left\|\Psi_{\pm,t}^{\varepsilon,\delta} - \varphi_{\pm,t}^{\varepsilon,\delta}\right\|_{L^2(\mathbb{R})} \leqslant \pm\frac{2}{\sqrt{\varepsilon}}\int_0^{\pm T} s^2\left\|y\,\tilde{v}_s^{\delta,\pm}(y)\,\mathbb{1}_{\pm y \leqslant -\frac{s^2}{2\sqrt{\varepsilon}}}\right\|_{L^2(\mathbb{R})} ds \tag{6.2.7}$$

after applying Proposition 6.1.2. To evaluate this integral, fix $\alpha = \frac{1}{17}$ and denote $\tau_\varepsilon = \varepsilon^{\frac{1}{4}-\alpha}$:

- For $t \in (-\tau_\varepsilon, \tau_\varepsilon)$, (6.2.7) gives

$$\begin{aligned}\sup_{t \in (-\tau_\varepsilon,\tau_\varepsilon)}\left\|\Psi_{\pm,t}^{\varepsilon,\delta} - \varphi_{\pm,t}^{\varepsilon,\delta}\right\|_{L^2(\mathbb{R})} &\leqslant \frac{2}{3}\frac{\tau_\varepsilon^3}{\sqrt{\varepsilon}}\left\|y\,\tilde{v}_t^{\delta,\pm}(y)\right\|_{L^{\infty}((-\tau_\varepsilon,\tau_\varepsilon),L^2(\mathbb{R}))} \\ &= \varepsilon^{\frac{1}{4}-3\alpha} K_\delta,\end{aligned} \tag{6.2.8}$$

  with $K_\delta > 0$ constant. The fact that $\left\|y\,\tilde{v}^{\delta,\pm}\right\|_{L^{\infty}((-\tau_\varepsilon,\tau_\varepsilon),L^2(\mathbb{R}))}$ is bounded comes from Remark 6.2.3.

- For the estimate for $t \in \Upsilon^\varepsilon = [-T, -\tau_\varepsilon] \cup [\tau_\varepsilon, T]$, remark that $\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}} \leqslant -\frac{\varepsilon^{-2\alpha}}{2}$ implies $|y|^{-5} \leqslant 2^5 \varepsilon^{10\alpha}$, then:

$$\left\| y\, v_t^{\delta,\pm}(y)\, \mathbb{1}_{\left\{\pm y \leqslant -\frac{t^2}{2\sqrt{\varepsilon}}\right\}} \right\|_{L^2(\mathbb{R})} \leqslant 2^5 \varepsilon^{10\alpha} \left\| y^6\, v_t^{\delta,\pm}(y) \right\|_{L^2(\mathbb{R})}.$$

Boundedness for the norm in last equation's right-hand side comes from the previous Remark 6.2.3.

Finally, form (6.2.7),

$$\begin{aligned} \sup_{t\in(-\tau_\varepsilon,\tau_\varepsilon)} \left\| \Psi_{\pm,t}^{\varepsilon,\delta} - \varphi_{\pm,t}^{\varepsilon,\delta} \right\|_{L^2(\mathbb{R})} &\leqslant \frac{2^6\, T^3}{3} \varepsilon^{10\alpha - \frac{1}{2}} \left\| y^6\, v^{\delta,\pm} \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))} \\ &= \varepsilon^{10\alpha-\frac{1}{2}} \tilde{K}_\delta \end{aligned} \tag{6.2.9}$$

for a constant $\tilde{K}_\delta > 0$.

Because of our choice of $\alpha = \frac{1}{17}$, both estimates (6.2.8) and (6.2.9) go to 0 with $\varepsilon \longrightarrow 0$, and we prove the proposition. □

So, in this section we saw the example of a case where the initial measure splits in two pieces, each one gliding to its side as in Figure 3.4.2, accordingly to the quantum distribution of mass along the x-axis.

Remark that there is no crossings at all. The part μ^- that goes to the left downwards did not come from the same side as μ^+, but from the very left. The portion that was in the right for $t < 0$ stays in the right all the time.

6.2.2 Measures crossing the singularity

Now, consider for $\eta \leqslant 0$ the Hamiltonian trajectories of $V(x) = -|x|$:

$$\begin{cases} \xi^\eta(t) = \eta \pm t \\ x^\eta(t) = \eta t \pm \frac{t^2}{2} \end{cases} \quad \text{for} \quad \pm\, \mathrm{t} \leqslant 0. \tag{6.2.10}$$

In this section, we will prove:

Proposition 6.2.4. *If $\Psi^{\varepsilon,\eta}$ is solution to the Schrödinger equation* (3.1.2) *with $V(x) = -|x|$ in $\mathbb{R}$, $\eta < 0$ and initial data*

$$\Psi_0^{\varepsilon,\eta}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} a\left(\frac{x}{\sqrt{\varepsilon}}\right) e^{\frac{i}{\varepsilon}\eta \cdot x},$$

with $a \in C_0^\infty(\mathbb{R})$, $\|a\|_{L^2(\mathbb{R})} = 1$, then the associated semiclassical measures are

$$\mu_t^\eta(x,\xi) = \delta(x - x^\eta(t)) \otimes \delta(\xi - \xi^\eta(t))$$

for any $t \in \mathbb{R}$.

Besides, if we take $\eta = -\varepsilon^\beta$ with $0 < \beta < \frac{1}{10}$, then the corresponding semiclassical measure will be, for $t \in \mathbb{R}$,

$$\mu_t(x,\xi) = \delta(x - x^0(t)) \otimes \delta(\xi - \xi^0(t)).$$

Proof. For the case with $\eta < 0$ constant, just apply Lemmata 6.2.7 and 6.2.9 ahead choosing $\beta = 0$. For the case $\eta = -\varepsilon^{\beta}$, same thing, but of course taking $0 < \beta < \frac{1}{10}$. □

Before we proceed to the lemmata, let us define $u^{\varepsilon,\eta}$ after (6.1.5) using the trajectories in (6.2.10), so as $u^{\varepsilon,\eta}$ satisfies the following system:

$$\begin{cases} i\partial_t u_t^{\varepsilon,\eta}(y) = -\frac{1}{2}\Delta u_t^{\varepsilon,\eta}(y) + \frac{1}{\varepsilon}R_t^{\varepsilon,\eta}(y)\; u_t^{\varepsilon,\eta}(y) \\ u_0^{\varepsilon,\eta}(y) = a(y). \end{cases}$$

We have:

Lemma 6.2.5. *Above, for* $t \neq 0$ *we have*

$$R_t^{\varepsilon,\eta}(y) = 2\left(x^{\eta}(t) + \sqrt{\varepsilon}y\right)\left(\mathbb{1}_{\{t<0\}}\mathbb{1}_{\left\{y<-\frac{x^{\eta}(t)}{\sqrt{\varepsilon}}\right\}} - \mathbb{1}_{\{t>0\}}\mathbb{1}_{\left\{y>-\frac{x^{\eta}(t)}{\sqrt{\varepsilon}}\right\}}\right) \tag{6.2.11}$$

and

$$\left|\frac{1}{\varepsilon}R_t^{\varepsilon,\eta}(y)\right| \leqslant \frac{2|y|}{\sqrt{\varepsilon}}\left(\mathbb{1}_{\{t<0\}}\mathbb{1}_{\left\{y<-\frac{x^{\eta}(t)}{\sqrt{\varepsilon}}\right\}} + \mathbb{1}_{\{t>0\}}\mathbb{1}_{\left\{y>-\frac{x^{\eta}(t)}{\sqrt{\varepsilon}}\right\}}\right). \tag{6.2.12}$$

Proof. Write down

$$\begin{aligned} \frac{1}{\varepsilon}R_t^{\varepsilon,\eta}(y) &= -\frac{1}{\varepsilon}\left(\left|x^{\eta}(t) + \sqrt{\varepsilon}y\right| - |x^{\eta}(t)| - \operatorname{sign}(x^{\eta}(t))\sqrt{\varepsilon}y\right) \\ &= -\frac{y}{\sqrt{\varepsilon}}\left(\frac{2\,x^{\eta}(t) + \sqrt{\varepsilon}y}{|x^{\eta}(t) + \sqrt{\varepsilon}y| + |x^{\eta}(t)|} - \operatorname{sign}(x^{\eta}(t))\right) \end{aligned}$$

and observe that $\operatorname{sign}(x^{\eta}(t)) = -\operatorname{sign}(t)$ for the trajectory in (6.2.10). □

Now, define

$$\tilde{v}_t^{\varepsilon,\eta}(y) = e^{-\frac{i}{\varepsilon}\int_0^t R_s^{\varepsilon,\eta}(y)ds}\, a(y) \tag{6.2.13}$$

and, given some small $\tau_{\varepsilon} \in (0, T)$, consider the following wave packet profile equation linked to the trajectory (6.2.10):

$$\begin{cases} i\partial_t v_t^{\varepsilon,\eta}(y) = -\frac{1}{2}\Delta v_t^{\varepsilon,\eta}(y) \\ v_{\pm\tau_\varepsilon}^{\varepsilon,\eta}(y) = \tilde{v}_{\pm\tau_\varepsilon}^{\varepsilon,\eta}(y) \end{cases} \quad \text{for} \quad t \in \Upsilon^{\varepsilon} = [-T, -\tau_{\varepsilon}] \cup [\tau_{\varepsilon}, T]. \tag{6.2.14}$$

Definition 6.2.6. *We will call* $\varphi^{\varepsilon,\eta}$ *the wave packet defined as in* (6.1.1) *for trajectory* (6.2.10)*, having profile* $\tilde{v}^{\varepsilon,\eta}$ *for* $t \in [-\tau_{\varepsilon}, \tau_{\varepsilon}]$ *and profile* $v^{\varepsilon,\eta}$ *otherwise.*

Lemma 6.2.7. *For* $\eta_{\varepsilon} = \eta\varepsilon^{\beta}$ *with* $\eta < 0$ *and* $0 \leqslant \beta < \frac{1}{10}$*, one has*

$$\lim_{\varepsilon \longrightarrow 0} \|\Psi^{\varepsilon,\eta_{\varepsilon}} - \varphi^{\varepsilon,\eta_{\varepsilon}}\|_{L^{\infty}([-T,T],L^2(\mathbb{R}))} = 0.$$

Proof. Let us treat the problem partitioning it in zones by choosing $\tau_{\varepsilon} = \varepsilon^{\alpha}$ with $\alpha > \beta$:

- $t \in [-\tau_{\varepsilon}, \tau_{\varepsilon}]$:
  Denote[2] $z^{\varepsilon} = u^{\varepsilon} - \tilde{v}^{\varepsilon}$; then $z_0^{\varepsilon}(y) = 0$,

$$i\partial_t z_t^{\varepsilon}(y) + \frac{1}{2}\Delta z_t^{\varepsilon}(y) - \frac{1}{\varepsilon}R_t^{\varepsilon}(y)\, z_t^{\varepsilon}(y) = -\frac{1}{2}\Delta\tilde{v}_t^{\varepsilon}(y)$$

[2] Since now η depends on ε, we will drop down the dependencies on η in order not to overcharge the notation. We will also let the dependency of the trajectories on ε implicit until it be crucial to take it into account.

and consequently

$$\begin{aligned}\frac{d}{dt}\,\|\, z_t^\varepsilon \,\|_{L^2(\mathbb{R})}^2 &= -2\,\mathrm{Im}\,\langle\, z_t^\varepsilon \,,\, \Delta \tilde{v}_t^\varepsilon \,\rangle_{L^2(\mathbb{R})} \\ &\leqslant 2\left|\langle\, \nabla u_t^\varepsilon \,,\, \nabla \tilde{v}_t^\varepsilon \,\rangle_{L^2(\mathbb{R})}\right| \\ &\leqslant \|\, \nabla u_t^\varepsilon \,\|_{L^2(\mathbb{R})}\,\|\, \nabla \tilde{v}_t^\varepsilon \,\|_{L^2(\mathbb{R})}\,.\end{aligned}$$

Given that ∇u^ε satisfies

$$i\partial_t\left(\nabla u_t^\varepsilon(y)\right) + \frac{1}{2}\Delta\left(\nabla u_t^\varepsilon(y)\right) - \frac{1}{\varepsilon} R_t^\varepsilon\,(y)\left(\nabla u_t^\varepsilon(y)\right) = \frac{1}{\varepsilon}\nabla R_t^\varepsilon\,(y)\,u_t^\varepsilon(y),$$

one can estimate, in the same way as in Proposition 6.1.2 (which enables us to avoid calculating R_t^ε at t = 0),

$$\begin{aligned}\|\, \nabla u_t^\varepsilon \,\|_{L^2(\mathbb{R})} &\leqslant \|\, \nabla a \,\|_{L^2(\mathbb{R})} + |t| \left\| \frac{1}{\varepsilon}\nabla R^\varepsilon\, u^\varepsilon \right\|_{L^\infty(\,]0,t[\,,L^2(\mathbb{R}))} \\ &\leqslant \|\, \nabla a \,\|_{L^2(\mathbb{R})} + \frac{2|t|}{\sqrt{\varepsilon}},\end{aligned}$$

the last line coming from quantum normalization and the facts that $\|u_t^\varepsilon\|_{L^2(\mathbb{R})} = 1$ is constant ($\|u_t^\varepsilon\|_{L^2(\mathbb{R})} = \|\Psi_t^\varepsilon\|_{L^2(\mathbb{R})}$) and

$$\frac{1}{\varepsilon}\,|\nabla R_t^\varepsilon\,(y)| = \frac{1}{\sqrt{\varepsilon}}\left|\frac{x(t)+\sqrt{\varepsilon}y}{|x(t)+\sqrt{\varepsilon}y|} - \mathrm{sign}\,(x(t))\right| \quad \text{for} \quad t \neq 0,$$

so $\left\|\frac{1}{\varepsilon}R_t^\varepsilon\right\|_{L^\infty(\mathbb{R})} \leqslant \frac{2}{\sqrt{\varepsilon}}$ for $t \in \,]\,0\,,t\,[\,.$

As a step aside, notice the following:

$$\nabla\tilde{v}_t^\varepsilon\,(y) = -i\tilde{v}_t^\varepsilon\,(y)\,\nabla\underbrace{\left(\frac{1}{\varepsilon}\int_0^t R_s^\varepsilon\,(y)\,ds\right)}_{I^\varepsilon(t,y)} + e^{-\frac{i}{\varepsilon}\int_0^t R_s^\varepsilon(y)ds}\,\nabla a(y).$$

Let us resume the main reasoning.

Taking into account the domain restrictions of R^ε (see (6.2.11)), for $\pm t < 0$ one must have satisfied the inequalities $\pm y < 0$ and $t^2 \pm 2\,\eta_\varepsilon\, t \pm 2\sqrt{\varepsilon}y < 0$ in order not to have R^ε null, which means that, for fixed y, t is comprised in $[-\varsigma(y), \varsigma(y)]$, where

$$\varsigma(y) = \eta_\varepsilon + \sqrt{\eta_\varepsilon^2 + 2\sqrt{\varepsilon}|y|} > 0 \tag{6.2.15}$$

is one of the roots of $\varsigma^2 - 2\,\eta_\varepsilon\,\varsigma - 2\sqrt{\varepsilon}y = 0$. Further, remark that $R_{\pm\varsigma(y)}^\varepsilon\,(y) = 0$; as a consequence,

$$I^\varepsilon(t,y) = \begin{cases} \frac{1}{\varepsilon}\int_0^t R_s^\varepsilon\,(y)\,ds & \text{if} \quad |t| < \varsigma(y) \\ \frac{1}{\varepsilon}\int_0^{\pm\varsigma(y)} R_s^\varepsilon\,(y)\,ds & \text{if} \quad \pm t \geqslant \varsigma(y), \end{cases} \tag{6.2.16}$$

which implies

$$\partial_y I^\varepsilon(t,y) = \begin{cases} \frac{2}{\sqrt{\varepsilon}}t & \text{if} \quad |t| < \varsigma(y) \\ \frac{2}{\sqrt{\varepsilon}}\varsigma(y) & \text{if} \quad t \geqslant \varsigma(y) \\ -\frac{2}{\sqrt{\varepsilon}}\varsigma(y) & \text{if} \quad t \leqslant -\varsigma(y). \end{cases} \tag{6.2.17}$$

Now, considering that $2\beta < \frac{1}{2}$, that $\eta_\varepsilon < 0$ and that there is $K > 0$ such that $|y| < K$, since within $\nabla \tilde{v}^\varepsilon$ we still have multiplying factors a and ∇a that are compactly supported in y, it can be made the estimative:

$$\varsigma(y) = \eta_\varepsilon + |\eta_\varepsilon| \left(1 + \frac{2\sqrt{\varepsilon}|y|}{\eta_\varepsilon^2}\right)^{\frac{1}{2}} \leqslant \frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|} K,$$

which in any case gives $|\partial_y I^\varepsilon(t,y)| \lesssim \frac{C_1}{|\eta_\varepsilon|}$ for some constant $C_1 > 0$, hence

$$\| \nabla \tilde{v}_t^\varepsilon \|_{L^2(\mathbb{R})} \lesssim \frac{C_1}{|\eta_\varepsilon|} \| a \|_{L^2(\mathbb{R})} = \frac{C_1}{|\eta_\varepsilon|}.$$

Finally, this results is a superior bound for $\|u_t^\varepsilon - \tilde{v}_t^\varepsilon\|_{L^2(\mathbb{R})}$ in $[-\tau_\varepsilon, \tau_\varepsilon]$; so, for a constant $C_2 > 0$:

$$\| z^\varepsilon \|^2_{L^\infty([-\tau_\varepsilon,\tau_\varepsilon],L^2(\mathbb{R}))} \lesssim C_2 \frac{\tau_\varepsilon}{|\eta_\varepsilon|} + C_1 \frac{\tau_\varepsilon^2}{\sqrt{\varepsilon}|\eta_\varepsilon|} \tag{6.2.18}$$

As $\alpha > \beta$ by assumption, the only additional constraint we need in order to have the bound above small when $\varepsilon \longrightarrow 0$ is:

$$2\alpha - \beta - \frac{1}{2} > 0. \tag{6.2.19}$$

- $t \in \Upsilon^\varepsilon = [-T, -\tau_\varepsilon] \cup [\tau_\varepsilon, T]$:

Hereafter denote $z^\varepsilon = u^\varepsilon - v^\varepsilon$. Now z^ε obeys to the equation

$$i\partial_t z_t^\varepsilon(y) + \left(\frac{1}{2}\Delta - \frac{1}{\varepsilon} R_t^\varepsilon(y)\right) z_t^\varepsilon(y) = \frac{1}{\varepsilon} R_t^\varepsilon(y)\, v_t^\varepsilon(y)$$

and, therefore,

$$\| z_t^\varepsilon \|_{L^2(\mathbb{R})} \leqslant \| z_{\pm\tau_\varepsilon}^\varepsilon \|_{L^2(\mathbb{R})} \pm \int_{\pm\tau_\varepsilon}^t \left\| \frac{1}{\varepsilon} R_s^\varepsilon\, v_s^\varepsilon \right\|_{L^2(\mathbb{R})} ds$$

according to t being positive or negative.

Recalling the trajectory defined in (6.2.10), the estimation in (6.2.12) and the fact that $\eta_\varepsilon < 0$, one has that R^ε is non-zero only in the region $|y| > \frac{|\eta_\varepsilon t|}{\sqrt{\varepsilon}} \geqslant \frac{|\eta_\varepsilon|\tau_\varepsilon}{\sqrt{\varepsilon}}$, so $\frac{1}{|y|} < \frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|\tau_\varepsilon}$; this gives

$$\begin{aligned} \left\| \frac{1}{\varepsilon} R_t^\varepsilon\, v_t^\varepsilon \right\|_{L^2(\mathbb{R})} &\leqslant \frac{2}{\sqrt{\varepsilon}} \| y\, v_t^\varepsilon \|_{L^2(\mathbb{R})} \\ &\leqslant \frac{2}{|\eta_\varepsilon|\tau_\varepsilon} \left(\frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|\tau_\varepsilon}\right)^k \left\| y^{k+2}\, v_t^\varepsilon \right\|_{L^2(\mathbb{R})}. \end{aligned}$$

Lemma 6.2.8. *For $t \in \Upsilon^\varepsilon$, $n, m \in \mathbb{N}_0$ and $\beta < \frac{1}{4}$, there exists $K_{n+m} > 0$ constant such that $\|y^n \nabla^m v_t^\varepsilon\|_{L^2(\mathbb{R})} \leqslant \frac{K_{n+m}}{|\eta_\varepsilon|^{n+m}}$.*

(The proof is postponed.)

As a conclusion, for ε small enough we have

$$\left\| \frac{1}{\varepsilon} R_t^\varepsilon \, v_t^\varepsilon \right\|_{L^2(\mathbb{R})} \leqslant \frac{2K_n}{|\eta_\varepsilon|^3 \tau_\varepsilon} \left(\frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|^2 \tau_\varepsilon} \right)^k ,$$

which carries the new constraint:

$$\frac{k}{2} - (k+1)\alpha - (2k+3)\beta > 0 \tag{6.2.20}$$

for some $k \in \mathbb{N}$.

The proposition is proven once we remark that for any $0 \leqslant \beta < \frac{1}{10}$, one can find a positive integer k such that both (6.2.19) and (6.2.20) will be satisfied for $\alpha > \beta$. □

Proof of Lemma 6.2.8. To evaluate $\|y^n v_t^\varepsilon\|_{L^2(\mathbb{R})}$, observe that by recurrence one can show that, for $n \in \mathbb{N}_0$,

$$i\partial_t \left(y^n v^\varepsilon \right) + \frac{1}{2} \Delta \left(y^n v^\varepsilon \right) = \frac{1}{2} n(n-1) y^{n-2} \, v^\varepsilon + n \, y^{n-1} \, \nabla v^\varepsilon$$

and, since $\nabla^m v^\varepsilon$ satisfies the same equation (6.2.14) as v^ε,

$$i\partial_t \left(y^n \nabla^m v^\varepsilon \right) + \frac{1}{2} \Delta \left(y^n \nabla^m v^\varepsilon \right) = \frac{1}{2} n(n-1) y^{n-2} \, \nabla^m v^\varepsilon + n \, y^{n-1} \, \nabla^{m+1} v^\varepsilon, \tag{6.2.21}$$

from where we have the estimation:

$$\begin{aligned} \|y^n \nabla^m v_t^\varepsilon\|_{L^2(\mathbb{R})} \leqslant \|y^n \nabla^m v_{\pm\tau_\varepsilon}^\varepsilon\|_{L^2(\mathbb{R})} &+ \frac{1}{2} n(n-1) T \left\| y^{n-2} \nabla^m v^\varepsilon \right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} \\ &+ nT \left\| y^{n-1} \nabla^{m+1} v^\varepsilon \right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} . \end{aligned}$$

The trick will be to transform the $L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)$ norms of the terms with $\nabla^m v^\varepsilon$ into $L^2(\mathbb{R})$ ones, so observe that we have

$$\begin{aligned} \left\| y^{n-2} \nabla^m v_t^\varepsilon \right\|_{L^2(\mathbb{R})} \leqslant \left\| y^{n-2} \nabla^m v_{\pm\tau_\varepsilon}^\varepsilon \right\|_{L^2(\mathbb{R})} &+ \frac{1}{2} (n-2)(n-3) T \left\| y^{n-4} \nabla^m v^\varepsilon \right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} \\ &+ (n-2) T \left\| y^{n-3} \nabla^{m+1} v^\varepsilon \right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} \end{aligned} \tag{6.2.22}$$

and, of course, that the right-hand side above also bounds $\left\| y^{n-2} \nabla^m v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$.

Repeating the steps above for the term $\left\| y^{n-4} \nabla^m v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$ that appears in (6.2.22), we will obtain an expression with the $L^2(\mathbb{R})$ norm $\left\| y^{n-4} \nabla^m v_{\pm\tau_\varepsilon}^\varepsilon \right\|_{L^2(\mathbb{R})}$ (as wished) and, additionally, the terms $\left\| y^{n-6} \nabla^m v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$ and $\left\| y^{n-5} \nabla^{m+1} v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$. Well, then we just repeat the same procedure for $\left\| y^{n-6} \nabla^m v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$, then for the term $\left\| y^{n-8} \nabla^m v^\varepsilon \right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$ that will appear, etc... and what we get is essentially

$$\|y^n \nabla^m v_t^\varepsilon\|_{L^2(\mathbb{R})} \leqslant \sum_{j=0}^{\left\lfloor \frac{n}{2} \right\rfloor} \left(c_{n,j}^{(1)} \left\| y^{n-2j} \nabla^m v_{\pm\tau_\varepsilon}^\varepsilon \right\|_{L^2(\mathbb{R})} + c_{n,j}^{(2)} \left\| y^{n-1-2j} \nabla^{m+1} v^\varepsilon \right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} \right), \tag{6.2.23}$$

with $c_{n,j}^{(1)}$ and $c_{n,j}^{(2)}$ appropriate coefficients.

Two things are remarkable in this formula. The first one is that all terms $y^{n-2j}\nabla^m v^\varepsilon_{\pm\tau_\varepsilon}$ have the same support (recall their definition, in (6.2.13) and (6.2.14)), which is the compact support of a. This bounds $|y|$ uniformly with respect to n, m, j and ε, implying that

$$\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} c^{(1)}_{n,j} \left\| y^{n-2j}\nabla^m v^\varepsilon_{\pm\tau_\varepsilon}\right\|_{L^2(\mathbb{R})} = d_{n,m}\left\|\nabla^m v^\varepsilon_{\tau_\varepsilon}\right\|_{L^2(\mathbb{R})},$$

where, again, $d_{n,m}$ is a suitable coefficient not depending on ε.

The second remarkable thing is that among the terms within the $L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)$ norms, the highest power of y that we find is $n-1$, and no more n, as in the beginning. This suggests that we may do the very same analysis for estimating each term $\left\|y^{n-1-2j}\nabla^{m+1}\right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))}$ in (6.2.23) and obtain estimates like

$$\begin{aligned}\left\|y^{n-1-2j}\nabla^{m+1}v^\varepsilon\right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)} &\leqslant d_{n-1-2j,m+1}\left\|\nabla^{m+1}v^\varepsilon_{\pm\tau_\varepsilon}\right\|_{L^2(\mathbb{R})} \\ &+ \sum_{l=0}^{\lfloor \frac{1}{2}(n-1-2j)\rfloor}\left\|y^{n-2-2(j+l)}\nabla^{m+2}v^\varepsilon\right\|_{L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)};\end{aligned}$$

again, the maximal power of y to appear inside the $L^\infty\left(\Upsilon^\varepsilon, L^2(\mathbb{R})\right)$ norms has been reduced by 1 with respect to the norm being estimated in the left-hand side. Whence, running recursively until we bring the maximal exponent down to 0, we will end up with:

$$\left\|y^n\nabla^m v^\varepsilon_t\right\|_{L^2(\mathbb{R})} \leqslant \sum_{j=0}^{n-1}\tilde{d}_j\left\|\nabla^{m+j}v^\varepsilon_{\pm\tau_\varepsilon}\right\|_{L^2(\mathbb{R})} + \tilde{d}_n\left\|\nabla^{m+n}v^\varepsilon\right\|_{L^\infty(\Upsilon^\varepsilon, L^2(\mathbb{R}))},$$

with ε-independent coefficients $\tilde{d}_j$. Finally, from equation 6.2.21, one knows that the norm $\|\nabla^{n+m}v^\varepsilon_t\|_{L^2(\mathbb{R})}$ is constant in time, so we can simplify even more the last estimation and have got:

$$\left\|y^n\nabla^m v^\varepsilon_t\right\|_{L^2(\mathbb{R})} \leqslant \sum_{j=0}^{n}\tilde{d}_j\left\|\nabla^{m+j}v^\varepsilon_{\pm\tau_\varepsilon}\right\|_{L^2(\mathbb{R})}. \tag{6.2.24}$$

Making use of (6.2.13) and the initial condition (6.2.14), let us calculate the remaining quantities:

$$\nabla^m v^\varepsilon_{\pm\tau_\varepsilon}(y) = e^{-\frac{i}{\varepsilon}\int_0^{\pm\tau_\varepsilon}R^\varepsilon_s(y)ds}\sum_{l=0}^{m}\begin{pmatrix} m \\ l\end{pmatrix}\nabla^{m-l}a(y)\sum_{\substack{\sigma\in\mathbb{N}_0^m \\ \sum_{s=1}^m s\sigma_s = l}}\left(c^\sigma\prod_{j=1}^m\left(\partial^j_y I^\varepsilon(\pm\tau_\varepsilon, y)\right)^{\sigma_j}\right),$$

where c^σ are complex coefficients.

The way for calculating the expression above is the following: if condition (6.2.20) is fulfilled, then we have $\alpha < \frac{1}{2}-\beta$, which causes τ_ε to be always greater than $|\varsigma(y)| \sim \frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|}$. Then, using (6.2.17), we get $\partial^{j+1}_y I^\varepsilon(\pm\tau_\varepsilon, y) = \pm\frac{2}{\sqrt{\varepsilon}}\partial^j_y\varsigma(y)$ for $j\in\mathbb{N}_0$, and, using (6.2.15) and being $\alpha > 2\beta$ (from (6.2.19) and the fact that $0\leqslant\beta<\frac{1}{10}$):

$$\frac{1}{\sqrt{\varepsilon}}\partial^{j+1}_y\varsigma(y) \sim \left(\frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|}\right)^j\frac{1}{|\eta_\varepsilon|^{j+1}};$$

thus, if we do the brutal majoration, $\frac{\sqrt{\varepsilon}}{|\eta_\varepsilon|} \lesssim 1$, one gets $\left|\partial_y^{j+2} I^\varepsilon(\pm\tau_\varepsilon, y)\right| \lesssim \frac{1}{|\eta_\varepsilon|^j}$ for all $j \in \mathbb{N}_0$, and also $I^\varepsilon(\pm\tau_\varepsilon, y) \sim \varsigma(y) \lesssim 1$. Additionally, we already had $\partial_y I^\varepsilon(\pm\tau_\varepsilon, y) \sim \frac{1}{|\eta_\varepsilon|}$, so even in the worst case one can always have the estimate

$$\partial_y^j I(\pm\tau^\varepsilon, a) \lesssim \frac{1}{|\eta_\varepsilon|^j},$$

which is, of course, far from optimal if $j \geqslant 2$ and just bad if $j = 0$, but fits in our purposes.

It follows that, for σ such that $\sum_{s=1}^m j\sigma_j = l$ and conveniently chosen constants K_j,

$$\prod_{j=1}^m \left(\partial_y^j I(\pm\tau_\varepsilon, y)\right)^{\sigma_j} \leqslant \frac{1}{|\eta_\varepsilon|^l} \prod_{j=1}^m K_j,$$

so $\left\|\nabla^m v^\varepsilon_{\pm\tau_\varepsilon}\right\|_{L^2(\mathbb{R})}$ will be dominated by a term of order $\frac{1}{|\eta_\varepsilon|^m}$ and, finally, inequality (6.2.24) will be bounded by a term of order $\frac{1}{|\eta_\varepsilon|^{n+m}}$, what we wanted to show. □

This completes the proposition's proof.

Lemma 6.2.9. *With $\eta_\varepsilon = \eta\varepsilon^\beta$, $\eta < 0$, the semiclassical measure associated with the family $(\varphi^{\varepsilon,\eta_\varepsilon})_{\varepsilon>0}$ is transported by a trajectory of shape* (6.2.10)*: $\left(x^0(t), \xi^0(t)\right)$ if $0 < \beta < \frac{1}{10}$, and $(x^\eta(t), \xi^\eta(t))$ if $\beta = 0$.*

Proof. The fact that $\varphi^{\varepsilon,\eta_\varepsilon}$ concentrates to a measure that follows the aimed path is not guaranteed by Lemma 6.1.1 since the initial data we inserted in the wave packet equation (6.2.14) is not ε-independent, as we required in Section 6.1. Let us then calculate the concentration of $\varphi^{\varepsilon,\eta_\varepsilon}$ indirectly.

To begin with, if conditions (6.2.19) and (6.2.20) are fulfilled, then $\tau_\varepsilon > \varsigma(y)$ and consequently, from (6.2.13), (6.2.15) and (6.2.16):

$$\tilde{v}^{\varepsilon,\eta_\varepsilon}_{\pm\tau_\varepsilon}(y) = e^{-\frac{i}{\varepsilon}\int_0^{\pm\varsigma(y)} R^\varepsilon_s(y)ds} a(y) = e^{-i\sqrt{\varepsilon}\left|\frac{y}{\eta_\varepsilon}\right|^3} e^{-i\left(\left(\frac{y}{\eta_\varepsilon}\right)^2 \mp \left|\frac{y}{\eta_\varepsilon}\right|\right)} a(y),$$

thus, setting $\hat{v}^\varepsilon_{\pm,0}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} \tilde{v}^{\varepsilon,\eta_\varepsilon}_{\pm\tau_\varepsilon}\left(\frac{x}{\sqrt{\varepsilon}}\right)$, one has

$$\hat{v}^\varepsilon_{\pm,0}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} a\left(\frac{x}{\sqrt{\varepsilon}}\right) f_1\left(\frac{x}{\eta_\varepsilon\sqrt{\varepsilon}}\right) f_2\left(\frac{\varepsilon^{\frac{1}{6}}x}{\eta_\varepsilon\sqrt{\varepsilon}}\right),$$

where $|f_1| = |f_2| = 1$ and ∇f_1 and ∇f_2 exist and are locally bounded almost everywhere in $\mathbb{R}$. These facts and standard symbolic calculus allow a straightforward calculation showing that $\hat{v}^\varepsilon_{\pm,0}$ concentrates to the measure $\mu_0^{\hat{v}^\varepsilon_\pm}(x,\xi) = \delta(x) \otimes \delta(\xi)$.

Now, define $\hat{v}^\varepsilon_\pm$ as the functions in $L^\infty(\mathbb{R}, L^2(\mathbb{R}))$ that satisfy the systems

$$\begin{cases} i\varepsilon\partial_t \hat{v}^\varepsilon_{\pm,t}(x) = -\frac{\varepsilon^2}{2}\Delta\hat{v}^\varepsilon_{\pm,t}(x) \\ \hat{v}^\varepsilon_{\pm,0}(x) = \frac{1}{\varepsilon^{\frac{1}{4}}}\tilde{v}^{\varepsilon,\eta_\varepsilon}_{\pm\tau_\varepsilon}\left(\frac{x}{\sqrt{\varepsilon}}\right); \end{cases}$$

it is possible to affirm that the semiclassical measures of $\hat{v}^\varepsilon_\pm$ will by carried by the flow $\Phi_t(x,\xi) = (x + t\,\xi, \xi)$, since by standard results (see the Introduction) they should obey to the usual Liouville equation (2.2.16) with a null potential. But because initially they are concentrated to the point $(0,0)$ in the phase space, we get $\mu_t^{\hat{v}_\pm^\varepsilon}(x,\xi) = \delta(x) \otimes \delta(\xi)$ for all $t \in \mathbb{R}$.

Well, for $\pm t \geqslant 0$, $\hat{v}_{\pm,t}^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{1}{4}}} v_{t\pm\tau_\varepsilon}^{\varepsilon,\eta_\varepsilon}\left(\frac{x}{\sqrt{\varepsilon}}\right)$, so observe that, for $\pm t \in [\tau_\varepsilon, T]$,

$$\varphi_t^{\varepsilon,\eta_\varepsilon}(x) = \hat{v}_{\pm,t\mp\tau_\varepsilon}^\varepsilon(x - x^{\eta_\varepsilon}(t))\, e^{\frac{i}{\varepsilon}[\xi^{\eta_\varepsilon}(t)\cdot(x - x^{\eta_\varepsilon}(t)) + S^{\eta_\varepsilon}(t)]};$$

consequently, by picking up a $b \in C_0^\infty(\mathbb{R}^2)$, one gets

$$\begin{aligned} \langle \mathrm{op}_\varepsilon(b)\, \varphi_t^{\varepsilon,\eta_\varepsilon}, \varphi_t^{\varepsilon,\eta_\varepsilon} \rangle_{L^2(\mathbb{R})} &= \left\langle \mathrm{op}_\varepsilon\left(b\left(x + x^{\eta_\varepsilon}(t), \xi + \xi^{\eta_\varepsilon}(t)\right)\right) \hat{v}_{\pm,t\mp\tau_\varepsilon}^\varepsilon, \hat{v}_{\pm,t\mp\tau_\varepsilon}^\varepsilon \right\rangle_{L^2(\mathbb{R})} \\ &= \left\langle \mathrm{op}_\varepsilon\left(b\left(x + x^{\eta_\varepsilon}(t), \xi + \xi^{\eta_\varepsilon}(t)\right)\right) \hat{v}_{\pm,t}^\varepsilon, \hat{v}_{\pm,t}^\varepsilon \right\rangle_{L^2(\mathbb{R})} + \mathcal{O}\left(\varepsilon^{\alpha-2\beta}\right), \end{aligned}$$

with the error coming from

$$\left\| \hat{v}_{\pm,t}^\varepsilon - \hat{v}_{\pm,t\mp\tau_\varepsilon}^\varepsilon \right\|_{L^2(\mathbb{R})} \leqslant \frac{\tau_\varepsilon}{2} \left\| \Delta v_{\pm\tau_\varepsilon}^\varepsilon \right\|_{L^2(\mathbb{R})} \leqslant K \frac{\tau_\varepsilon}{|\eta_\varepsilon|^2} = K\varepsilon^{\alpha-2\beta},$$

where $K > 0$ is constant and we used Lemma 6.2.8. If $\beta = 0$, then $\eta_\varepsilon = \eta$ is constant and we get, for $t \in [-T,T] \setminus \{0\}$,

$$\operatorname{sc\,lim} \langle \mathrm{op}_\varepsilon(b)\, \varphi_t^{\varepsilon,\eta}, \varphi_t^{\varepsilon,\eta} \rangle_{L^2(\mathbb{R})} = \langle \delta(x) \otimes \delta(\xi), b(x + x^\eta(t), \xi + \xi^\eta(t)) \rangle_{\mathbb{R}^2},$$

which also holds for $t = 0$ due to the initial condition for $\varphi^{\varepsilon,\eta}$, implying that

$$\mu_t^{\varphi^{\varepsilon,\eta}}(x,\xi) = \delta(x - x^\eta(t)) \otimes \delta(\xi - \xi^\eta(t))$$

for all $t \in [-T,T]$.

If $0 < \beta < \frac{1}{10}$, we can still have

$$\langle \mathrm{op}_\varepsilon(b)\, \varphi_t^\varepsilon, \varphi_t^\varepsilon \rangle_{L^2(\mathbb{R})} = \left\langle \mathrm{op}_\varepsilon\left(b\left(x + x^0(t), \xi + \xi^0(t)\right)\right) \hat{v}_{\pm,t}^\varepsilon, \hat{v}_{\pm,t}^\varepsilon \right\rangle_{L^2(\mathbb{R})} + o(1) + \mathcal{O}\left(\varepsilon^{\alpha-2\beta}\right),$$

and now the error $o(1)$ comes from the difference between calculating b with the trajectories $(x^{\eta_\varepsilon}(t), \xi^{\eta_\varepsilon}(t))$ or the with "limit" path $(x^0(t), \xi^0(t))$, which must be negligible in compact times for ε small enough, given that b is smooth and the flow that defines the trajectories is stable in the region where we are. Since it is possible to choose $\alpha > 2\beta$ within conditions (6.2.19) and (6.2.20), an argument similar to the previous one gives

$$\mu_t^{\varphi^{\varepsilon,\eta_\varepsilon}}(x,\xi) = \delta(x - x^0(t)) \otimes \delta(\xi - \xi^0(t))$$

for all $t \in [-T,T]$ when $0 < \beta < \frac{1}{10}$. □

Remark 6.2.10. All results in this section also work taking $\eta > 0$ and swapping t negative for positive and conversely in the definition of the trajectories (6.2.10).

Hence, we have found that it is possible that a particle arrive into the singularity from the up left or from the down right and that it continue to the other side down or up, as partially indicated in Figure 3.4.1(b). Moreover, we also proved that the wave packet approximation is valid for the non-smooth trajectories indicated in Figure 3.4.3 (and for the reverse ones not indicated in the picture).

Chapter 7

The exact solutions

Remark. Contrarily to the rest of this thesis, in this chapter we will use the Physics standard notation

$$\langle \psi_1 \,,\, \psi_2 \rangle_{L^2(M)} = \int_M \overline{\psi_1(x)}\, \psi_2(x)\, dx$$

for the inner product in $L^2(M)$ or for some extension of it (in which case we will drop the label $_{L^2(M)}$ down).

7.1 The case $V(x) = +|x|$

In this section we give an exact solution to the one-dimensional Schrödinger equation (3.1.2) with potential $V(x) = |x|$.

Introducing the *Ansatz* $\Psi^\varepsilon(t, x) = \varphi(x)\, T(t)$ in (3.1.2), we are given $T_E(t) = e^{-\frac{i}{\varepsilon}Et}$ and $\hat{H}^\varepsilon \varphi = E\varphi$; more explicitly:

$$-\frac{\varepsilon^2}{2}\partial_x^2 \varphi(x) + |x|\, \varphi(x) = E\varphi(x)\,, \tag{7.1.1}$$

where $E \in \mathbb{R}$ is some constant to be fixed later that stands for the quantum state's energy.

Replacing $\varphi(x) = \phi(y)$, with

$$\begin{array}{lcl} y = \sqrt[3]{\frac{2}{\varepsilon^2}}\,(x - E) & \text{for} & x > 0 \\ y = \sqrt[3]{\frac{2}{\varepsilon^2}}\,(-x - E) & & x < 0, \end{array} \tag{7.1.2}$$

one gets, for any $x \neq 0$:

$$\partial_y^2 \phi(y) - y\phi(y) = 0, \tag{7.1.3}$$

whose solutions are superpositions of the Airy functions Ai and Bi[91]. Because we want them to decrease to 0 at infinity so as the final solution be $L^2(\mathbb{R})$, we are left with only the first kind of Airy function, Ai, so for each possible E we have:

$$\begin{array}{lcl} \varphi_E(x) = \alpha_E^+ \operatorname{Ai}\left(\sqrt[3]{\frac{2}{\varepsilon^2}}\,(x - E)\right) & \text{for} & x > 0 \\ \varphi_E(x) = \alpha_E^- \operatorname{Ai}\left(\sqrt[3]{\frac{2}{\varepsilon^2}}\,(-x - E)\right) & & x < 0, \end{array}$$

where $\alpha_E^{\pm}$ are complex coefficients. Imposing continuity for φ_E at $x = 0$:

$$\alpha_E^+ = \alpha_E^- \neq 0 \qquad \text{or} \qquad E_{2n+1}^{\varepsilon} = -\lambda_{2n+1}\sqrt[3]{\frac{\varepsilon^2}{2}} \;\text{ so }\; \varphi_E(0) = 0,$$

where λ_{2n+1} is the n-th zero of the Airy function. Imposing continuity for $\partial_x\varphi_E$ at $x = 0$:

$$\alpha_E^+ = -\alpha_E^- \neq 0 \qquad \text{or} \qquad E_{2n}^{\varepsilon} = -\lambda_{2n}\sqrt[3]{\frac{\varepsilon^2}{2}} \;\text{ so }\; \partial_x\varphi_E(0) = 0,$$

where λ_{2n} is the n-th zero of the derivative of the first kind Airy function.

Therefore, choosing $\alpha_n^{\varepsilon} > 0$ in a suitable way, the normalized eigenstates for the system's Hamiltonian have the form:

$$\varphi_n^{\varepsilon}(x) = \alpha_n^{\varepsilon}\left(\mathbb{1}_{\{x\geqslant 0\}} - \mathbb{1}_{\{x<0\}}\right)^n \operatorname{Ai}\left(\sqrt[3]{\frac{2}{\varepsilon^2}}\,|x| + \lambda_n\right) \qquad \forall n \in \mathbb{N}_0.$$

The self-adjointness of $\hat{H}^{\varepsilon}$ with domain $H^2(\mathbb{R})$ assures that the general solution for this equation is a superposition of these eigenstates:

$$\Psi^{\varepsilon}(t,x) = \sum_{n\in\mathbb{N}_0} c_n^{\varepsilon}\,\varphi_n^{\varepsilon}(x)e^{-\frac{i}{\sqrt[3]{2\varepsilon}}\lambda_n t}, \tag{7.1.4}$$

with suitable complex coefficients c_n^{ε} chosen so as to satisfy the initial condition $\Psi^{\varepsilon}(0,x) = \Psi_0^{\varepsilon}(x)$, which can be obtained applying the orthogonality relations $\langle\varphi_n^{\varepsilon}, \varphi_m^{\varepsilon}\rangle_{L^2(\mathbb{R})} = \delta_{n,m}$:

$$c_n^{\varepsilon} = \int_{\mathbb{R}} \overline{\varphi_n^{\varepsilon}(x)}\Psi_0^{\varepsilon}(x)dx.$$

To conclude the analysis, remark that λ_n does not depend on ε nor on any other parameter, so it is possible to describe the distribution of the energy levels E_n^{ε}. The first ones are known explicitly from the computed values of λ_n and, for $n \geqslant N$ with N large enough, one can use the asymptotic formulæ for the Airy function and its derivative[91] to obtain:

$$E_{2n}^{\varepsilon} \approx \frac{1}{2}\sqrt[3]{9\varepsilon^2\pi^2\left(k_n + \frac{1}{4}\right)^2} \qquad \text{and} \qquad E_{2n+1}^{\varepsilon} \approx \frac{1}{2}\sqrt[3]{9\varepsilon^2\pi^2\left(k_n + \frac{3}{4}\right)^2},$$

where $(k_n)_{n\geqslant N}$ is some sequence such that $k_{n+1} = k_n + 1$.

Observe that they form an infinite countable set bounded from below by a ground state E_0^{ε}, do not accumulate to any value as $n \longrightarrow \infty$ (so arbitrarily high energies are allowed) and are such that $E_n^{\varepsilon} < E_m^{\varepsilon}$ for any $n < m$ in $\mathbb{N}_0$, as it is usual for linked states.

7.2 The case $V(x) = -|x|$

7.2.1 Confined states

Now we shall solve the Schrödinger equation for $V(x) = -|x|$. Before analysing our actual case of interest, in $L^2(\mathbb{R})$, let us solve (3.1.2) inside the compact $[-1, 1]$ with Cauchy homogeneous conditions, which will enlighten some technical issues that we will face in the free case.

We proceed as we have already done previously, inserting $\Psi^\varepsilon(x,t) = \varphi(x)T(t)$ in (3.1.2) in order to obtain $T_E(t) = e^{-\frac{i}{\varepsilon}Et}$ and equation (7.1.1), from which we get (7.1.3) through a variable change similar to (7.1.2), but swapping x by $-x$.

Nevertheless, in the present situation it is not going to be possible to discard Bi, the second type of Airy function, based on arguments of decay. Hence, φ is going to be a linear combination of these functions:

$$\begin{aligned} \varphi_E(x) &= \alpha_E^+ \operatorname{Ai}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(x+E)\right) + \beta_E^+ \operatorname{Bi}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(x+E)\right) && \text{for} \quad x>0 \\ \varphi_E(x) &= \alpha_E^- \operatorname{Ai}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(-x+E)\right) + \beta_E^- \operatorname{Bi}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(-x+E)\right) && \phantom{\text{for}} \quad x<0, \end{aligned}$$

and the conditions for continuity of φ and $\partial_x\varphi$ at $x=0$ read:

$$\begin{cases} \left(\alpha_E^+ - \alpha_E^-\right)\operatorname{Ai}\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) + \left(\beta_E^+ - \beta_E^-\right)\operatorname{Bi}\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) = 0 \\ \left(\alpha_E^+ + \alpha_E^-\right)\operatorname{Ai}'\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) + \left(\beta_E^+ + \beta_E^-\right)\operatorname{Bi}'\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) = 0, \end{cases}$$

where Ai′ and Bi′ are the derivatives of Ai and Bi and $\alpha_E^\pm, \beta_E^\pm \in \mathbb{C}$. We can choose two linearly independent solutions that satisfy these equalities for any E, one even (P) and the other odd (I):

(7.2.1)

$$\begin{aligned} \varphi_E^{\varepsilon,P}(x) &= \operatorname{Bi}'\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right)\operatorname{Ai}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(|x|+E)\right) - \operatorname{Ai}'\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right)\operatorname{Bi}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(|x|+E)\right) \\ \varphi_E^{\varepsilon,I}(x) &= \left(\mathbb{1}_{\{x\geqslant 0\}} - \mathbb{1}_{\{x<0\}}\right)\left(\operatorname{Bi}\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right)\operatorname{Ai}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(|x|+E)\right) - \operatorname{Ai}\left(-E\sqrt[3]{\tfrac{2}{\varepsilon^2}}\right)\operatorname{Bi}\left(-\sqrt[3]{\tfrac{2}{\varepsilon^2}}(|x|+E)\right)\right). \end{aligned}$$

Finally, imposing the boundary condition $\varphi_E^{\varepsilon,P,I}(1) = \varphi_E^{\varepsilon,P,I}(-1) = 0$ for the even (P) and the odd (I) solutions, we find out that the only allowed values of E are:

$$\begin{aligned} E_{2n}^\varepsilon &= -\lambda_{2n}^\varepsilon \sqrt[3]{\tfrac{\varepsilon^2}{2}} && \text{for} \quad \varphi_E^P \\ E_{2n+1}^\varepsilon &= -\lambda_{2n+1}^\varepsilon \sqrt[3]{\tfrac{\varepsilon^2}{2}} && \phantom{\text{for}} \quad \varphi_E^I, \end{aligned}$$

where λ_{2n}^ε and $\lambda_{2n+1}^\varepsilon$ are respectively the n-th zeros of the functions:

$$\begin{aligned} f_\varepsilon^P(\eta) &= \operatorname{Bi}'(\eta)\operatorname{Ai}\left(\eta - \sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) - \operatorname{Ai}'(\eta)\operatorname{Bi}\left(\eta - \sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) \\ f_\varepsilon^I(\eta) &= \operatorname{Bi}(\eta)\operatorname{Ai}\left(\eta - \sqrt[3]{\tfrac{2}{\varepsilon^2}}\right) - \operatorname{Ai}(\eta)\operatorname{Bi}\left(\eta - \sqrt[3]{\tfrac{2}{\varepsilon^2}}\right). \end{aligned}$$

Choosing a proper α_n^ε, the normalized eigenstates of $\hat{H}^\varepsilon$ in this case are given by:

$$\begin{aligned} \varphi_n^\varepsilon(t,x) = \alpha_n^\varepsilon \left(\mathbb{1}_{\{x\geqslant 0\}} - \mathbb{1}_{\{x<0\}}\right)^n \Bigg(&\operatorname{Bi}^{(1-n/2)}(\lambda_n^\varepsilon)\operatorname{Ai}\left(\lambda_n^\varepsilon - \sqrt[3]{\frac{2}{\varepsilon^2}}|x|\right) \\ &-\operatorname{Ai}^{(1-n/2)}(\lambda_n^\varepsilon)\operatorname{Bi}\left(\lambda_n^\varepsilon - \sqrt[3]{\frac{2}{\varepsilon^2}}|x|\right)\Bigg) \qquad \forall n \in \mathbb{N}_0, \end{aligned}$$

where we defined $n/2 = \frac{1}{2}\left[1-(-1)^n\right]$, which is 0 or 1 depending on n being even or odd.

Again, $\hat{H}^\varepsilon$ being self-adjoint on $H^2([-1,1])$ assures that the general solution will be a superposition of these eigenstates with suitable coefficients:

$$\Psi^\varepsilon(t,x) = \sum_{n\in\mathbb{N}_0} e^{-\frac{i}{\sqrt[3]{2\varepsilon}}\lambda_n^\varepsilon t}\varphi_n^\varepsilon(x)\left\langle \varphi_n^\varepsilon, \Psi_0^\varepsilon\right\rangle_{L^2([-1,1])}. \tag{7.2.2}$$

Concerning the energy levels, in practice the first values of μ_n^ε can be numerically computed with a simple integration for the differential system obeyed by f_ε^P and f_ε^I. Posing $\omega_\varepsilon = \sqrt[3]{\frac{2}{\varepsilon^2}}$:

$$\begin{cases} \partial_\eta^2 f_\varepsilon^P(\eta) + \omega_\varepsilon f_\varepsilon^P(\eta) = f_\varepsilon^I(\eta) + 2\eta\partial_\eta f_\varepsilon^I(\eta) \\ \partial_\eta^2 f_\varepsilon^I(\eta) + \omega_\varepsilon f_\varepsilon^I(\eta) = -2\partial_\eta f_\varepsilon^P(\eta). \end{cases}$$

The result is in Figure 7.2.1. For higher energies (in absolute value), we have the asymptotic formulæ obtained from the asymptotic expansions for Ai and Bi[91]:

$$\text{for } \eta \longrightarrow \infty : \quad \begin{array}{l} f_\varepsilon^I(\eta) \approx \frac{1}{2\pi\sqrt{\eta}} e^{\omega_\varepsilon \sqrt{\eta}} \\ f_\varepsilon^P(\eta) \approx \frac{1}{2\pi} e^{\omega_\varepsilon \sqrt{\eta}} \end{array} \tag{7.2.3}$$

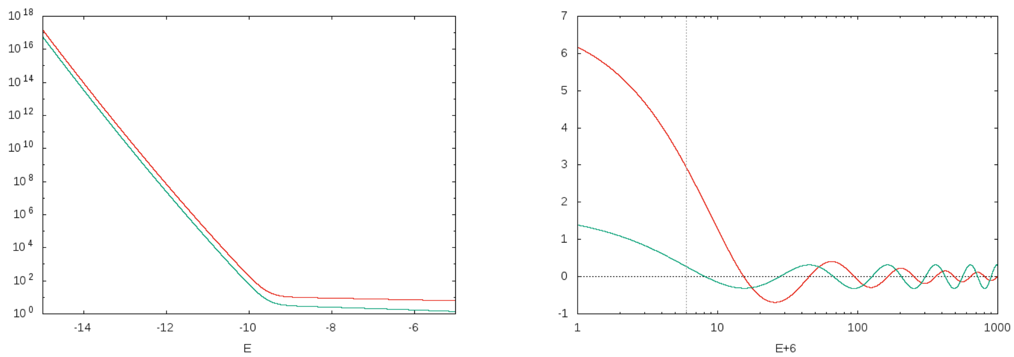
and

$$\text{for } \eta \longrightarrow -\infty : \quad \begin{array}{l} f_\varepsilon^I(\eta) \approx \frac{1}{\pi\sqrt{\eta}} \sin\left(\omega_\varepsilon\sqrt{-\eta}\right) \\ f_\varepsilon^P(\eta) \approx \frac{1}{\pi} \cos\left(\omega_\varepsilon\sqrt{-\eta}\right), \end{array} \tag{7.2.4}$$

They inform us that either f_ε^P and f_ε^I will not be zero for η big enough, or, in other terms, that the system has a ground energy state E_0. Conversely, for η too negative, the functions oscillate more or less like the trigonometric ones, thus for $n \geqslant N$ sufficiently large we can estimate:

$$E_{2n} \approx \frac{\varepsilon^2\pi^2}{2}\left(k_n + \frac{1}{2}\right)^2 \qquad \text{and} \qquad E_{2n+1} \approx \frac{\varepsilon^2\pi^2}{2}\left(k_n + 1\right)^2,$$

where $(k_n)_{n \geqslant N}$ is some suitable sequence such that $k_{n+1} = k_n + 1$.



(a) Exponential tendency for $E \ll 0$.

(b) Oscillatory tendency for $E \gg 0$.

Figure 7.2.1: Graphics for f^P (green) and f^I (red) as functions of $E = -\eta$ simulated for $\omega_\varepsilon = 1$. The graphic in (b) reproduces closely the asymptotes expected from (7.2.4); in (a) the functions' growth is clearly exponential, though the effect of the square root $\sqrt{-E}$ in (7.2.3) is not evident due to scaling restrictions.

As before, the set of eigenvalues is countable, lower bounded, ordered like $E_n < E_m$ for any $n < m$ in $\mathbb{N}_0$, non-accumulating and allows arbitrarily large energies, which is characteristic for confined states.

7.2.2 Free states

In solving (3.1.2) in $L^2(\mathbb{R})$ with $V(x) = -|x|$, we will incur in typical difficulties for free states, like the fact that $\hat{H}^\varepsilon$ will not have eigenvalues nor eigenstates and its (essential) spectrum will be continuous.

Indeed, we begin as in last section until we get, for each $E \in \mathbb{R}$, the two independent solutions (7.2.1). There, we could apply the Cauchy boundary conditions and obtain a discretization of choices for E. Here, this is not possible and, worse, the solutions to equation (7.1.1) (which was a genuine eigenvalue equation in the precedent cases) are not even $L^2(\mathbb{R})$ functions, so not acceptable answers to the quantum problem.

However, from the Weyl criterion (see [105], Problem 6.18 in particular) we deduce that the spectrum of $\hat{H}^\varepsilon$ is essential and coincides with $\mathbb{R}$; alternatively, the Shnol theorem[94] gives that the spectrum of $\hat{H}^\varepsilon$ is $\mathbb{R}$, since for any $E \in \mathbb{R}$ the solutions $\varphi_E^{\varepsilon,P}$ and $\varphi_E^{\varepsilon,I}$ are sub-exponential.

Furthermore, define $\varphi_E^\varepsilon = \alpha_E^{\varepsilon,P}\varphi_E^{\varepsilon,P} + i\alpha_E^{\varepsilon,I}\varphi_E^{\varepsilon,I}$, where $\alpha_E^{\varepsilon,P,I}$ are constants to be discussed in Remark 7.2.2 ahead. These are generalized eigenfunctions of $\hat{H}^\varepsilon$ with generalized eigenvalue E ([23, 24, 94]), in the sense that φ_E^ε is in the dual $\mathcal{H}_-$ of some Hilbert space $\mathcal{H}_+$ dense in $L^2(\mathbb{R})$ and, for any $\psi \in \mathcal{H}_+ \cap D\left(\hat{H}^\varepsilon\right)$:

$$\left\langle \varphi_E^\varepsilon, (\hat{H}^\varepsilon - E)\psi \right\rangle = 0. \tag{7.2.5}$$

In our case, since for any $E \in \mathbb{R}$ we have $\|\varphi_E^\varepsilon(\,\cdot\,)\|_\infty < \infty$, we may pick up any $\delta > 0$ and choose $\mathcal{H}_+ = \mathcal{F}\left(H^{\frac{1}{2}+\delta}(\mathbb{R})\right)$ and $\mathcal{H}_- = \mathcal{F}\left(H^{-\left(\frac{1}{2}+\delta\right)}(\mathbb{R})\right)$ (the images through the Fourier transform of these respective Sobolev spaces).

Besides, from the theorem of expansion in terms of generalized eigenfunctions[24, 94], the function $\mathcal{H}_+ \ni \psi \longmapsto \tilde{\psi} \in L^2(\mathbb{R})$ given by

$$\tilde{\psi}(E) = \langle \varphi_E^\varepsilon, \psi \rangle = \int_{\mathbb{R}} \overline{\varphi_E^\varepsilon(x)}\psi(x)dx \tag{7.2.6}$$

is well-posed and extends to a unitary operator $U \in \mathcal{L}\left(L^2(\mathbb{R}^d)\right)$.

Remark 7.2.1. Define $\mathcal{H} = \left\{\psi \in \mathcal{H}_+ : \tilde{\psi} \in \mathcal{H}_+\right\}$. Consequently, for $\psi \in \mathcal{H}$, we have:

$$\psi = \int_{\mathbb{R}} \varphi_E^\varepsilon \langle \varphi_E^\varepsilon, \psi \rangle \, dE; \tag{7.2.7}$$

observe that $\mathcal{H}$ is dense in $L^2(\mathbb{R})$ for it contains the Schwartz space[1], so although the above formula is not strictly correct for $\Psi \in L^2(\mathbb{R})$ in general, we may still employ it to stand for $\Psi = U^*U\Psi$, if we bear in mind that it must be understood along a strong limiting approximation $\Psi = \lim \psi_n$, with $\psi_n \in \mathcal{H}$ for all $n \in \mathbb{N}$.

In the same sense, the resolution of the identity

$$\mathbb{1} = \int_{\mathbb{R}} |\varphi_E^\varepsilon\rangle \langle \varphi_E^\varepsilon| \, dE \tag{7.2.8}$$

[1] Indeed, if $\psi \in \mathcal{S}(\mathbb{R})$, it follows from (7.2.5) and (7.2.6) that $E \longmapsto E^k\tilde{\psi}(E) = U\left((\hat{H}^\varepsilon)^k\psi\right)$ is $L^2(\mathbb{R})$ for any integer $k > 0$, so $\tilde{\psi}$ is rapidly decreasing and consequently is in $\mathcal{H}_+$.

holds for $L^2(\mathbb{R})$, and the spectral decomposition

$$\hat{H} = \int_R E \left|\varphi_E^\varepsilon\right\rangle \left\langle\varphi_E^\varepsilon\right| dE \tag{7.2.9}$$

can be used for doing functional calculus on the whole $\mathcal{L}\left(L^2(\mathbb{R})\right)$ (since any bounded Borelian function of $\hat{H}$ is a bounded operator, which allows us to take the necessary limits).

Remark 7.2.2. From equation (7.2.7), it is clear that we must have, in the sense of distributions in $\mathcal{H}$,

$$\int_{\mathbb{R}} \varphi_{E'}^\varepsilon(x)\overline{\varphi_E^\varepsilon(x)}dx = \delta\left(E - E'\right),$$

which fixes the choices for the constants $\alpha_E^{\varepsilon,P}$ and $\alpha_E^{\varepsilon,I}$. In particular, these constants must decrease fast enough as $E \longrightarrow \infty$ in order to attenuate the growth of $\|\varphi_E^\varepsilon(\,\cdot\,)\|_\infty$, so as the identity above can hold.

Therefore, in view of the general solution $\Psi^\varepsilon(t,\cdot) = e^{-\frac{i}{\varepsilon}t\hat{H}}\Psi_0^\varepsilon$, we use (7.2.9) to calculate

$$e^{-\frac{i}{\varepsilon}t\hat{H}} = \int_{\mathbb{R}} e^{-\frac{i}{\varepsilon}tE} \left|\varphi_E^\varepsilon\right\rangle \left\langle\varphi_E^\varepsilon\right| dE,$$

which carries

$$\Psi^\varepsilon(t,x) = \int_{\mathbb{R}} e^{-\frac{i}{\varepsilon}tE}\varphi_E^\varepsilon(x) \left\langle\varphi_E^\varepsilon, \Psi_0^\varepsilon\right\rangle dE \tag{7.2.10}$$

in the limiting sense of Remark 7.2.1, $\Psi_0^\varepsilon = \lim \psi_n$ with $\psi_n \in \mathcal{H}$. Otherwise, in a more rigorous expression:

$$\Psi^\varepsilon(t,\cdot) = U^* e^{-\frac{i}{\varepsilon}t(\,\cdot\,)} U \Psi_0^\varepsilon(\,\cdot\,),$$

where U is the extension to $L^2(\mathbb{R})$ of the function $\mathcal{H}_+ \ni \psi \longmapsto \tilde{\psi} \in L^2(\mathbb{R})$ given in (7.2.6).

Remark 7.2.3. The calculations above are similar to what we have done in the previous cases. From (7.2.8) we are able to decompose the $L^2(\mathbb{R})$ solution Ψ^ε of (3.1.2) as

$$\Psi^\varepsilon(t,x) = \int_{\mathbb{R}} \alpha_E^\varepsilon(t)\varphi_E^\varepsilon(x)dE,$$

where $\alpha_E^\varepsilon(t) = \left\langle\varphi_E^\varepsilon, \Psi^\varepsilon(t,\cdot)\right\rangle$. In order to satisfy the Schrödinger equation, however, one should have, formally,

$$\left(i\varepsilon\partial_t - E\right)\alpha_E^\varepsilon(t) = \left\langle\varphi_E^\varepsilon, \left(i\varepsilon\partial_t - E\right)\Psi^\varepsilon(t,\cdot)\right\rangle = \left\langle\varphi_E^\varepsilon, \left(\hat{H}^\varepsilon - E\right)\Psi^\varepsilon(t,\cdot)\right\rangle \stackrel{!}{=} 0,$$

which would carry

$$\alpha_E^\varepsilon(t) = e^{-\frac{i}{\varepsilon}Et}\alpha_E^\varepsilon \qquad \text{with} \qquad \alpha_E^\varepsilon = \left\langle\varphi_E^\varepsilon, \Psi_0^\varepsilon\right\rangle,$$

and the final solution (7.2.10).

This calculation is more than merely formal, since step (!) above may be understood as an extension of (7.2.5) to the whole $L^2(\mathbb{R})$, made possible by the fact that the application $\psi \longmapsto \left\langle\varphi_E^\varepsilon, \left(\hat{H}^\varepsilon - E\right)\psi\right\rangle$ coincides with the continuous operator 0 all over the dense subspace $\mathcal{H}_+$.

7.3 A comment on the classical solutions for $V(x) = -|x|$

Now let us have a glance on the supposedly classical system with $V(x) = -|x|$. The trajectories can be seen in Figure 3.1.1(b), where it becomes apparent that the flow is ill-defined at the origin. When coming from the right-hand side below, there seems to be two alternative trajectories after reaching $x = 0$ with zero momentum: going back to the right upwards, or crossing to the left downwards. Actually there are infinitely many possibilities, because between arriving to the origin and leaving it a particle could stay there, say, 17 minutes, nothing, or the eternity; not to consider the other infinitely many trajectories coming from the left-hand side above or those standing on the origin since the beginning and later starting to move at some moment.

Were we discussing perfectly punctual particles climbing a slope with a perfectly sharp peak – and were we perfectly classical physicists –, we could argue that in order to preserve *determinism* it would be necessary that all trajectories attaining $x = 0$ with $\xi = 0$ take to the same way thereafter. Nevertheless, classical mechanical systems should also present *reversibility*, thus a possible solution for it should work with time counted regressively as well. For a reversible system, two trajectories on the phase space cannot be continued by the same path, otherwise the reversed system would not be deterministic, nor can they stop "in the middle of the way" like the branches of parabola coming from the up-left or down-right and stopping at $(0, 0)$. Clearly, in this situation determinism and reversibility are incompatible[2].

We could, however, consider a weakened version of determinism. Let us imagine that it were possible to determine the future and past trajectories of a particle given not only its position and momentum at an initial instant t_0, but also these same data during all a previous duration $(t_0 - \varepsilon, t_0]$. In this case, one could introduce a selection principle based on the particle's history. For example, when examining a particle at the pick: if it were climbing from the left, let us say that it would be determined to cross the origin and continue down to the right; the opposite if it were coming from the right; if it were already at the top, then it would keep laying there.

Such a system is (historically) deterministic and reversible, further to time homogeneous. In some sense it is also space homogeneous, considering that the mirrored system would behave under the same rules as the straight one. Other selection principles could be thought of, but it could never happen that a moving particle stopped not to move any more. Should this be the case, after a time $t_0 + 2\varepsilon$ we would lose the ability to reconstruct the particle's past, once we would not know the time it reached the peak, and for the reversed system it would be impossible to predict its future behaviour, being impossible to say at which moment the particle would begin its movement (though certain to begin).

If Theorem 3.4.1 dismisses the possibility to reconstruct a classical theory based on selection principles that could be recovered from the quantum one, it is interesting to note that we have not presented the case of a Wigner measure that really changes from the exterior flow to the flow on the singular manifold, *i.e.*, we did not present any particle moving and then stopping at the peak, or stopped thereon and then spontaneously starting to move.

Preliminary calculations gave the impression that, at least for the case of wave packets

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[2]And we have not even considered *space and time homogeneity*: the particle would need to stop at the top not to choose one side over the other, but it would not be allowed to stop there, since for the reversed system this would mean that a particle that lasted at rest for some while would be able to start moving at some preferred instant even under a constant potential.

similar to those that we analysed, this would not be possible. This is a point to be remembered in the Conclusion and Perspectives in the end of this thesis.

Part III

Impure Periodic Potentials

Chapter 8

Presenting the problem – periodic potentials with impurities

Part III of this thesis was a joint work with Dr. Clotilde Fermanian and Dr. Fabricio Macià, published independently in [32].

8.1 The dynamics of an electron in a crystal and effective mass theory

The dynamics of an electron in a crystal in the presence of impurities is described by a wave function $\Psi(t,x)$ that solves the Schrödinger equation

$$\begin{cases} i\hbar\partial_t\Psi(t,x) = -\frac{\hbar^2}{2m}\Delta\Psi(t,x) + Q_{\text{per}}(x)\,\Psi(t,x) + Q_{\text{ext}}(x)\Psi(t,x) \\ \Psi(0,x) = \Psi_0(x). \end{cases} \tag{8.1.1}$$

The potential Q_{per} is periodic with respect to some lattice in $\mathbb{R}^d$ and describes the interactions between the electron and the crystal. The external potential Q_{ext} takes into account the effects of impurities on the otherwise perfect crystal. Here, $\hbar$ denotes the Planck's constant and m is the electronic mass. In many cases of physical interest, the ratio between the lattice's characteristic length and the mean spacing scale of variation of Q_{ext} can be considered very small, *i.e.*, the impurities can be seen as very dispersed inside the crystal's structure.

Denote this ratio by ε. After performing a suitable change of units and rescaling the external potential and the wave function (see for instance [96]), the Schrödinger equation becomes:

$$\begin{cases} i\partial_t\psi^\varepsilon(t,x) = -\frac{1}{2}\Delta\psi^\varepsilon(t,x) + \frac{1}{\varepsilon^2}V_{\text{per}}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon(t,x) + V(x)\psi^\varepsilon(t,x) \\ \psi^\varepsilon(0,x) = \psi_0^\varepsilon(x), \end{cases} \tag{8.1.2}$$

where the potential V_{per} is periodic with respect to a fixed lattice in $\mathbb{R}^d$, which will be assumed $\mathbb{Z}^d$ for the sake of simplicity.

In this context, the theory of effective mass consists in showing that, under suitable assumptions on the initial data ψ_0^ε, the solutions of (8.1.2) can be approximated for ε small by those of a simpler Schrödinger equation, the *effective mass equation*, which is of the form:

$$i\partial_t \phi(t,x) = -\frac{1}{2} M\partial_x \cdot \partial_x \phi(t,x) + V(x)\phi(t,x), \tag{8.1.3}$$

with some initial datum to be discussed later.

Above, M is a $d \times d$ matrix called the *effective mass tensor*. This quantity is obtainable experimentally and can be used to study the effects of impurities on the electronic dynamics. Both the questions of finding the initial conditions for which the corresponding solutions of (8.1.2) converge in a suitable sense to solutions to the effective mass equation and that of clarifying the dependence of M on the sequence of initial data ψ_0^ε have been extensively studied in the literature[6, 19, 22, 64, 96].

Besides, another scaling limit that has been widely studied in this field is the *semiclassical limit*[5, 20, 27, 37, 56, 58, 65, 93, 96], which deals with the behaviour as $\varepsilon \longrightarrow 0$ of solutions to the semiclassical Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t v^\varepsilon(t,x) = -\frac{\varepsilon^2}{2}\Delta v^\varepsilon(t,x) + V_{\text{per}}\left(\frac{x}{\varepsilon}\right) v^\varepsilon(t,x) + \varepsilon^2 V(x) v^\varepsilon(t,x) \\ v^\varepsilon(0,x) = \psi_0^\varepsilon(x), \end{cases} \tag{8.1.4}$$

whose characteristic wave lengths are comparable to ε. Again, the interested reader can consult [96] for details on the well known derivation of (8.1.4) from (8.1.1). Anyway, it is easy to check that the solutions to (8.1.2) and (8.1.4) are related through the identity

$$\psi^\varepsilon(t,x) = v^\varepsilon\left(\frac{t}{\varepsilon}, x\right), \tag{8.1.5}$$

so, at least formally, one should be able to recover the effective mass equation (8.1.3) by performing the semiclassical limit $\varepsilon \longrightarrow 0$ in (8.1.4) simultaneously with $\frac{t}{\varepsilon} \longrightarrow +\infty$.

Remark 8.1.1. When the periodic potential is absent, this type of simultaneous limit, combining high frequencies $\varepsilon \longrightarrow 0$ and long times $t \sim t_\varepsilon \longrightarrow +\infty$ is relevant if one wants to understand the behaviour of solutions of (8.1.4) beyond the Ehrenfest time[10, 78, 80]. Also, again when $V_{\text{per}} = 0$, the change of time scale (8.1.5) transforms the semiclassical equation (8.1.4) into the non-semiclassical one (this is, with $\varepsilon = 1$), making it possible to derive results on the long time dynamics of the ordinary Schrödinger equation via this scaling limit[11, 12, 14, 77]. The reader can consult the survey articles [13, 79] and the introductory lecture notes [76] for additional details and references about this approach.

Our goal in this part of the thesis is to apply the aforementioned point of view to the effective mass theory by studying the asymptotic behaviour of position densities $|\psi^\varepsilon|^2$. Nevertheless, unlike in Part II here the potentials also depend on the semiclassical parameter ε, which will require us to use a technique that, so as to say, separates the effects of the periodic and the non-periodic potentials, *i.e.*, separates the normal electron's behaviour in the lattice from the perturbation it suffers from the impurities.

8.2 The Bloch-Floquet decomposition

This kind of analysis of Schrödinger operators with periodic potentials can be traced back to the works by Floquet[51] on ordinary differential equations with periodic coefficients, and by Bloch[25], who developed a spectral theory of periodic Schrödinger operators in the context of solid state physics. As we will see, the Bloch-Floquet theory also applies to perturbed periodic Hamiltonian operators

$$\hat{H} = -\frac{\varepsilon^2}{2}\Delta_x + V_{\text{per}}\left(\frac{x}{\varepsilon}\right) + \varepsilon^2 V(x),$$

in which we are presently interested[1].

The idea is based on the assumption that the solutions of (8.1.2) depend on both the "slow" x and the "fast" $\frac{x}{\varepsilon}$ variables, leading to the following Ansatz on the form of the solutions ψ^ε of (8.1.2):

$$\psi^\varepsilon(t,x) = U^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right), \tag{8.2.1}$$

where $U^\varepsilon(t,x,y)$ is assumed to be $\mathbb{Z}^d$-periodic with respect to the variable y and, therefore, can be identified to a function defined on $\mathbb{R}\times\mathbb{R}^d\times\mathbb{T}^d$, $\mathbb{T}^d$ denoting the torus $\mathbb{R}^d/\mathbb{Z}^d$. One easily checks that U^ε must solve the following equation:

$$\begin{cases} i\varepsilon^2\partial_t U^\varepsilon(t,x,y) = -\frac{1}{2}(\varepsilon\partial_x + \partial_y)^2 U^\varepsilon(t,x,y) + V_{\text{per}}(y)U^\varepsilon(t,x,y) + \varepsilon^2 V(x)U^\varepsilon(t,x,y) \\ U^\varepsilon(0,x,y) = \tilde{\psi}_0^\varepsilon(x,y), \end{cases} \tag{8.2.2}$$

where the initial condition is to be interpreted in terms of the natural embedding $L^2(\mathbb{R}^d_x) \hookrightarrow L^2(\mathbb{R}^d_x\times\mathbb{T}^d_y)$, $\tilde{\psi}_0^\varepsilon(x,y) = \psi_0^\varepsilon(x)\ \forall y\in\mathbb{T}^d$. The fact that ψ^ε must be given by (8.2.1) follows from the unicity of the solutions to the initial value problem (8.1.2).

Now, concerning the Fourier transform of U^ε with respect to x,

$$\hat{U}^\varepsilon(t,\xi,y) = \int_{\mathbb{R}^d} e^{-i\xi\cdot x}\, U^\varepsilon(t,x,y)\,dx,$$

the equation that it satisfies involves the following family of operators acting on $\mathbb{Z}^d$-periodic functions[2]

$$P(\varepsilon\xi) = \frac{1}{2}\left(\varepsilon\xi - i\partial_y\right)^2 + V_{\text{per}}, \quad \xi\in\mathbb{R}^d. \tag{8.2.3}$$

As it is usual for Schrödinger-like operators on compact domains, $P(\xi)$ is self-adjoint on $L^2(\mathbb{T}^d)$; it has therefore a compact resolvent and a non-decreasing sequence of eigenvalues called *Bloch energies*,

$$\lambda_1(\xi) \leqslant \lambda_2(\xi) \leqslant \cdots \leqslant \lambda_n(\xi) \leqslant \cdots \underset{n\to\infty}{\longrightarrow} +\infty,$$

associated to an orthonormal basis of $L^2(\mathbb{T}^d)$ consisting of eigenfunctions $\varphi_n(\xi,\cdot)$ called *Bloch waves*,

$$P(\xi)\varphi_n(\xi,y) = \lambda_n(\xi)\varphi_n(\xi,y) \quad \text{for } y\in\mathbb{T}^d.$$

Moreover, the Bloch energies $\lambda_n(\xi)$ are $2\pi\mathbb{Z}^d$-periodic[3], whereas the Bloch waves satisfy

$$\varphi_n(\xi+2\pi k, y) = e^{-2\pi i k\cdot y}\varphi_n(\xi,y) \quad \forall k\in\mathbb{Z}^d.$$

[1]See for instance [69, 70, 71, 98] and the references therein, or [59, 64, 92] for results in the semiclassical context.

[2]Alternatively, one can simply check that $\hat{H}\psi^\varepsilon = \left(P(\varepsilon\partial_x) + V\right)U^\varepsilon|_{y=\frac{x}{\varepsilon}}$.

[3]This follows from the fact that for every $k\in\mathbb{Z}^d$, the operator $P(\xi+2\pi k)$ is unitary equivalent to $P(\xi)$ since $P(\xi+2\pi k) = e^{-2\pi i k\cdot y}P(\xi)e^{2\pi i k\cdot y}$.

Remark 8.2.1. It is proved in [110] that the Bloch energies λ_n are continuous and piecewise analytic functions[4] of $\xi \in \mathbb{R}^d$, and that the Bloch waves can be chosen in such a way that there exists a subset $\mathcal{Z}$ of the domain $\mathcal{B} = [-\pi, \pi)^d$ (called *Brillouin zone*) of zero Lebesgue measure such that each function $\xi \longmapsto \varphi_n(\xi, \cdot\,)$ is analytic in $\mathcal{B}\backslash\,\mathcal{Z}$. If the multiplicity of the family of eigenvalues $(\lambda_n(\xi))_{\xi\in\mathbb{R}^d}$ is constant, then λ_n is globally analytic; further, it will be possible to find an orthonormal eigenbasis consisting of functions whose dependence on ξ is also analytic.

Naturally, the spectral structure of $P(\varepsilon\xi)$ leads to the representation:

$$\hat{U}^\varepsilon(t,\xi,y) = \sum_{n\in\mathbb{N}} \varphi_n(\varepsilon\xi,y)\hat{U}^\varepsilon_n(t,\xi) \quad \text{with} \quad \hat{U}^\varepsilon_n(t,\xi) = \int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi,y)}\,\hat{U}^\varepsilon(t,\xi,y)dy$$

pointwisely in ξ, or, at least formally:

$$U^\varepsilon(t,x,y) = \sum_{n\in\mathbb{N}} \varphi_n(\varepsilon\partial_x,y)U^\varepsilon_n(t,x) \tag{8.2.4}$$

with

$$U^\varepsilon_n(t,x) = \int_{\mathbb{T}^d} \varphi_n(\varepsilon\partial_x,y)^*\,U^\varepsilon(t,x,y)dy, \tag{8.2.5}$$

where, for each $y \in \mathbb{T}^d$ and $n \in \mathbb{N}$, $\varphi_n(\varepsilon\partial_x, y)$ is the pseudodifferential operator of symbol $\xi \longmapsto \varphi_n(\,\cdot\,, y)$ defined in (2.1.1), and $\varphi_n(\varepsilon\partial_x, y)^*$ is its adjoint.

Equation (8.2.4) is called the *Bloch-Floquet decomposition* of U^ε, and its terms in (8.2.5) are the *Bloch modes* ([55, 59]). It is thus clear that the aimed solution ψ^ε can be formally given as

$$\psi^\varepsilon(t,x) = \sum_{n\in\mathbb{N}} \varphi_n\left(\varepsilon\partial_x, \frac{x}{\varepsilon}\right) U^\varepsilon_n(t,x), \tag{8.2.6}$$

so the only thing that still remains to be obtained are the Bloch modes U^ε_n. The precise sense in which the series in (8.2.4) converges will be presented ahead in Proposition 10.2.11, whereas the sum in (8.2.6) will be shown in equation (10.2.18) to converge in $L^2(\mathbb{R}^d)$ for each $t \in \mathbb{R}$, if some requirements on U^ε are fulfilled.

Well, since U^ε solves (8.2.2), we will be able to prove with a calculation analogous to that in Lemma 10.2.12:

Proposition 8.2.2. *For each $n \in \mathbb{N}$, the functions U^ε_n satisfy:*

$$U^\varepsilon_n(t,\cdot\,) = u^\varepsilon_n(t,\cdot\,) + \mathcal{O}(\varepsilon|t|) \quad \text{in } L^2(\mathbb{R}^d), \tag{8.2.7}$$

where u^ε_n are the solutions to:

$$\begin{cases} i\varepsilon^2\partial_t u^\varepsilon_n(t,x) = \lambda_n(\varepsilon\partial_x)u^\varepsilon_n(t,x) + \varepsilon^2 V(x)u^\varepsilon_n(t,x) \\ u^\varepsilon_n(0,x) = \int_{\mathbb{T}^d} \varphi_n(\varepsilon\partial_x,y)^*\tilde{\psi}^\varepsilon_0(x,y)dy. \end{cases} \tag{8.2.8}$$

[4] In the real analytic sense that they allow an expansion in terms of power series within the compacts of $\mathbb{R}^d$.

This is an adiabatic result, in the sense that it guarantees that the time evolution of each Bloch mode will be independent of the other modes up to a small error in $L^2(\mathbb{R}^d)$ norm that further disappears in the semiclassical limit.

In short, the solutions of (8.1.2) can be decomposed as a countable superposition of waves whose dependence on the fast variable is given by the Bloch waves, while the profiles u_n^ε describing (approximatively) the dependence on the slow variable are given by a time evolution (8.2.8) whose dispersion involves the corresponding Bloch energy. Consequently, we will be supposed to analyse the concentration of quantities $|u_n^\varepsilon|^2$, which will be done in Chapter 9, and then to somehow transpose them to $|\psi^\varepsilon|^2$, in Chapter 10. this approach follows the guidelines in [10, 12, 77]. Let us briefly describe them in the next sections.

8.3 Lacks of mass dispersion

As the previous discussion shows, one of the main steps in understanding the asymptotic behaviour as $\varepsilon \longrightarrow 0$ of solutions to the Schrödinger equation (8.1.2) relies on the analysis of solutions to an equation of the form:

$$\begin{cases} i\varepsilon^2\partial_t u^\varepsilon(t,x) = \lambda(\varepsilon\partial_x)u^\varepsilon(t,x) + \varepsilon^2 V(x)u^\varepsilon(t,x) \\ u^\varepsilon(0,x) = u_0^\varepsilon(x), \end{cases} \tag{8.3.1}$$

which ceases to be dispersive as soon as λ has non-zero critical points $\nabla\lambda(\xi) = 0$. Notice that this is always the case for Bloch energies, as they are periodic in ξ.

One of the consequences of a dispersive time evolution is regularizing the high frequency effects caused by the concentration of initial data that arise when keeping $\varepsilon\xi \neq 0$ constant when $\varepsilon \longrightarrow 0$, what in many cases has been made precise by establishing smoothing estimates[5] for the family of solutions u^ε[21, 35, 66, 68, 102, 107].

Consequently, the equation's lack of dispersiveness should cause a lack of regularization for the Bloch modes. In Remark 8.3.3 below, we will give a tiny insight of how, in the presence of critical points, some of these high frequency anomalies persist after evolving the initial data through (8.3.1).

These results are of independent interest, so we will expose them separately in Theorems 8.3.1 and 8.3.4, where we will completely describe the asymptotic behaviour of densities $|u^\varepsilon|^2$ associated to a bounded sequence $(u^\varepsilon)_{\varepsilon>0}$ of solutions to (8.3.1) by giving an explicit procedure to compute all accumulation points of $|u^\varepsilon|^2$ (in the weak topology) at any time, by just starting from the sequence of initial data u_0^ε.

Let us consider the following hypotheses:

H0 The sequence u_0^ε is uniformly bounded in $L^2(\mathbb{R}^d)$ and ε-oscillating, in the sense that its energy is concentrated on frequencies of order at most $\frac{1}{\varepsilon}$:

$$\limsup_{\varepsilon\to 0} \int_{\|\xi\|>\frac{R}{\varepsilon}} |\hat{u}_0^\varepsilon(\xi)|^2\, d\xi \underset{R\to\infty}{\longrightarrow} 0. \tag{8.3.2}$$

This assumption is necessary if we are to obtain the limit measures of $|u^\varepsilon|^2$ by projecting Wigner measures of u^ε over the space of positions, as explained in Chapter 2, equations (2.2.6) and (2.2.7).

[5] Generally, a smoothing estimate for $\Psi \in L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^d)\right)$ is an inequality of type $\|\Psi\|_{L^1\left(\Upsilon, H^s(\mathbb{R}^d)\right)} \leqslant C_\Upsilon \|\Psi_0\|_{L^2(\mathbb{R}^d)}$ for some $s > 0$, where $C_\Upsilon > 0$ is a constant for each $\Upsilon \subset \mathbb{R}$ compact.

H1 $V \in C^\infty(\mathbb{R}^d)$ is bounded together with its derivatives, and $\lambda \in C^\infty(\mathbb{R}^d)$ grows at most polynomially, *i.e.* there exist $C, N > 0$ such that:

$$|\lambda(\xi)| \leq C(1+|\xi|)^N \quad \forall \xi \in \mathbb{R}^d.$$

These requirements settle us on a comfortable frame of Schrödinger problems and might be weakened "on demand" depending on the concrete situations, provided that one does not infringe basic restrictions, like having under-quadratic potentials.

w-H2 The set

$$\Lambda = \left\{ \xi \in \mathbb{R}^d : \nabla\lambda(\xi) = 0 \right\}$$

is a submanifold of $\mathbb{R}^d$ of codimension $0 < p \leq d$ and the Hessian $\nabla^2\lambda$ is of maximal rank over Λ. Moreover, each connected component of Λ is compact.

Last hypothesis can be replaced by a stronger version that yields a simpler result:

s-H2 All critical points of λ are non-degenerate, *i.e.*, $\nabla^2\lambda(\xi)$ is a non-degenerate quadratic form for every $\xi \in \Lambda$. This implies that $p = d$ and, therefore, that Λ is a discrete set[6] in $\mathbb{R}^d$.

The necessity of at least **w-H2** will be made clear in Section 11.2, Chapter 11, where we will give examples of distinct behaviours that the concentrated measures can present if the Hessian of λ is not of full rank over Λ. In short, the effective mass results are about the operator-valued measure in the two-microlocal decomposition of the Wigner measure; assumptions **s-H2** or **w-H2** assure us that the measure in sphere will be null, so we will be left solely with this operator term obeying to effective mass equations.

Theorem 8.3.1. *Suppose that the family of initial data* $(u_0^\varepsilon)_{\varepsilon>0}$ *verifies* **H0** *and denote by* u^ε *the corresponding solutions of* (8.3.1). *Suppose in addition that* **H1** *is verified and that all critical points of* λ *are non-degenerate (***s-H2***).*

Then, there exists a sequence $(\varepsilon_k)_{k\in\mathbb{N}}$ *tending to* 0 *such that, for every* $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, *the following holds:*

$$\lim_{k\longrightarrow\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|u^{\varepsilon_k}(t,x)|^2 dxdt = \sum_{\xi_0\in\Lambda} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|u_{\xi_0}(t,x)|^2 dxdt, \tag{8.3.3}$$

where u_{ξ_0} *solves the Schrödinger equation with effective mass:*

$$\begin{cases} i\partial_t u_{\xi_0}(t,x) = -\frac{1}{2}\nabla^2\lambda(\xi_0)\partial_x \cdot \partial_x u_{\xi_0}(t,x) + V(x)u_{\xi_0}(t,x) \\ u_{\xi_0}(0,\cdot) = \mathrm{w}\lim_{k\to\infty} \left(e^{-\frac{i}{\varepsilon_k}\xi_0\cdot x} u_0^{\varepsilon_k} \right), \end{cases} \tag{8.3.4}$$

this $L^2(\mathbb{R}^d)$ *weak limit being unique.*

Finally, if $\Lambda = \emptyset$*, then the right-hand side of* (8.3.3) *is equal to zero.*

Remark 8.3.2. Since $L^2(\mathbb{R}^d)$ is reflexive, the weak and the weak-$*$ topologies thereon coincide, which assures the existence of weak limits for the family $\left(e^{-\frac{i}{\varepsilon}\xi_0\cdot x}u_0^\varepsilon\right)_{\varepsilon>0}$, given the Banach-Alaoglou theorem. Above, the unicity comes from the fact that we choose sequences $(\varepsilon_k)_{k\in\mathbb{N}}$ with the very purpose to get the particular limits $u_\xi|_{t=0}$ this family may give, so the concentration of u^ε may happen in as many different ways as there are different weak limits. This should become clear during the theorem's proof.

[6]If moreover one has that λ is $2\pi\mathbb{Z}^d$-periodic, which is the situation when λ is a Bloch energy, then this set is finite modulo $\mathbb{Z}^d$.

Remark 8.3.3. Let us now illustrate how Theorem 8.3.1 raises obstructions to the validity of smoothing estimates in the presence of non-zero critical points (although such estimates remain still valid away from the critical points[99]).

Assume that there exists a non-zero $\xi_0 \in \Lambda$ and take a family $(u^\varepsilon)_{\varepsilon>0}$ of solutions to (8.3.1) with initial data $u_0^\varepsilon = e^{\frac{i}{\varepsilon}\xi_0 \cdot x}\theta(x)$, where $\theta \in C_0^\infty(\mathbb{R}^d)$ is such that $\|\theta\|_{L^2(\mathbb{R}^d)} = 1$. Assume further that, for any $t \in \mathbb{R}$, $(u_t^\varepsilon)_{\varepsilon>0}$ tends weakly to zero in $L^2(\mathbb{R}^d)$. Theorem 8.3.1 states that the limit of the densities $|u^\varepsilon|^2$ is precisely $|u_{\xi_0}|^2$, which is not identically zero, since here we have $u_{\xi_0}(0,\cdot\,) = \theta \neq 0$; consequently, there exists $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$ such that:

$$\lim_{k\longrightarrow\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|u^{\varepsilon_k}(t,x)|^2 dxdt \neq 0. \tag{8.3.5}$$

On the other hand, we have:

$$\begin{aligned} \left|\int_{\mathbb{R}^d} \phi(t,x)|u^\varepsilon(t,x)|^2 dx\right| &= \left|\int_{\|\xi\|\leqslant R} \hat{\phi}_t * \hat{u}_t^\varepsilon(\xi)\,\overline{\hat{u}_t^\varepsilon(\xi)}d\xi + \int_{\|\xi\|>R} \frac{1}{\langle\xi\rangle^s}\hat{\phi}_t * \hat{u}_t^\varepsilon(\xi)\overline{\langle\xi\rangle^s\,\hat{u}_t^\varepsilon(\xi)}d\xi\right| \\ &\leqslant |\langle K_{\phi_t}u_t^\varepsilon, u_t^\varepsilon\rangle| + \frac{1}{R^s}\|\phi\|_{L^\infty(\mathbb{R}\times\mathbb{R}^d)}\|u_0^\varepsilon\|_{L^2(\mathbb{R}^d)}\|u_t^\varepsilon\|_{H^s(\mathbb{R}^d)}, \end{aligned}$$

where K_{ϕ_t} is a compact operator on $L^2(\mathbb{R}^d)$. Since the solutions $u^\varepsilon(t,\cdot\,)$ tend weakly to 0 for all $t \in \mathbb{R}$, one knows that $\langle K_\phi u_t^\varepsilon, u_t^\varepsilon\rangle \longrightarrow 0$ as $\varepsilon \longrightarrow 0$; therefore, if a smoothing estimate of the form $\|u^\varepsilon\|_{L^1\left(\Upsilon, H^s(\mathbb{R}^d)\right)} \leqslant C_\Upsilon\|u_0^\varepsilon\|_{L^2(\mathbb{R}^d)}$ held uniformly in ε for some $s > 0$, we would have:

$$\left|\lim_{k\longrightarrow\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|u^{\varepsilon_k}(t,x)|^2 dxdt\right| \leqslant \mathcal{O}\left(\frac{1}{R^s}\right).$$

The choice of R being arbitrarily large, the left hand side above would need to be null for every $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, a contradiction with (10.2.17).

The result obtained when the non-degeneracy of the critical points is replaced by the weaker condition **w-H2** is similar, but then it comes up in a continuous version, which will require some geometric preliminaries. For instance, the sum over the discrete critical points will be replaced by an integral over the cotangent bundle of Λ, and (8.3.4) becomes a Heisenberg equation for a time-dependent family of operators acting on functions over the manifold's conormal bundle.

So, define the cotangent bundle of Λ as:

$$T^*\Lambda = \{(x,\xi) \in \mathbb{R}^d \times \Lambda \,:\, x \in T_\xi^*\Lambda\},$$

and the conormal bundle of Λ as the union of those linear subspaces that are normal to Λ within $\mathbb{R}^d$:

$$N^*\Lambda = \{(y,\xi) \in \mathbb{R}^d \times \Lambda \,:\, y \in N_\xi^*\Lambda = (T_\xi^*\Lambda)^\perp\}.$$

This is in nothing different from the usual definitions of $T^*\Lambda$ and of $N^*\Lambda$ by quotienting its fibres, $N_\xi^* = {T_\xi^*\mathbb{R}^d}/{T_\xi^*\Lambda}$, and the use of the cotangent and conormal bundles instead of the tangent and the normal ones is justified by the fact that we will be working on submanifolds of the phase space.

Besides, every point $x \in \mathbb{R}^d$ can be uniquely written as $x = z + y$, where $z \in T^*_\xi\Lambda$ and $y \in N^*_\xi\Lambda$. Thus, given a function $\phi \in L^\infty(\mathbb{R}^d)$, we define the multiplication operator $m_\phi(z,\xi) \in \mathcal{L}\left(L^2\left(N^*_\xi\Lambda\right)\right)$ by:

$$m_\phi(z,\xi)\psi(y) = \phi(y+z)\psi(y) \quad \forall\psi \in L^2\left(N^*_\xi\Lambda\right).$$

Note as well that **w-H2** implies that, for every $\xi \in \Lambda$, the Hessian $\nabla^2\lambda(\xi)$ is an invertible operator on $N^*_\xi\Lambda$.

Theorem 8.3.4. *Let $(u_0^\varepsilon)_{\varepsilon>0}$ be a sequence of initial data satisfying* **H0** *and denote by u^ε the corresponding solutions of* (8.3.1)*. If* **H1** *and* **w-H2** *hold, then there exists a sequence $(\varepsilon_k)_{k\in\mathbb{N}}$ tending to* 0*, a positive measure $\gamma \in \mathcal{M}(T^*\Lambda)$ and a measurable family of self-adjoint, positive, trace-class operators*

$$\mathfrak{M}_0 : T^*\Lambda \ni (z,\xi) \longmapsto \mathfrak{M}_0(z,\xi) \in \mathcal{L}\left(L^2(N^*_\xi\Lambda)\right), \quad \mathrm{tr}_{L^2\left(N^*_\xi\Lambda\right)}\mathfrak{M}_0(z,\xi) = 1,$$

such that, for every $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, one has:

$$\lim_{k\longrightarrow\infty}\int_{\mathbb{R}\times\mathbb{R}^d}\phi_t(x)|u^{\varepsilon_k}(t,x)|^2dxdt = \int_{\mathbb{R}\times T^*\Lambda}\mathrm{tr}_{L^2\left(N^*_\xi\Lambda\right)}\left(m_{\phi_t}(z,\xi)\,\mathfrak{M}(t,z,\xi)\right)\gamma(dz,d\xi)dt, \tag{8.3.6}$$

where the $C\left(\mathbb{R},\mathcal{L}\left(L^2(N^*_\xi\Lambda)\right)\right)$ function $t \longmapsto \mathfrak{M}(t,z,\xi)$ solves the following Heisenberg equation with effective mass:

$$\begin{cases} i\partial_t\,\mathfrak{M}(t,z,\xi) = \left[-\frac{1}{2}\nabla^2\lambda(\xi)\partial\cdot\partial + m_V(z,\xi)\,,\,\mathfrak{M}(t,z,\xi)\right] \\ \mathfrak{M}(0,z,\xi) = \mathfrak{M}_0(z,\xi). \end{cases} \tag{8.3.7}$$

Here, $M_0 = \mathfrak{M}_0\gamma$ is the operator-valued two-microlocal measure of the family $(u_0^{\varepsilon_k})_{k\in\mathbb{N}}$ over Λ.

Remark 8.3.5. As in Remark 8.3.2, the measure γ and the family of operators $\mathfrak{M}_0$ only depend on the sequence $(\varepsilon_k)_{k\in\mathbb{N}}$, which is actually chosen in function of the possible limiting microlocal measures one can have. Furthermore, observe that γ and $\mathfrak{M}$ are respectively the scalar measure and the operator-valued function into which the operator-valued microlocal measure decomposes according to the Radon-Nikodym theorem; see Remark 9.1.4 ahead.

Remark 8.3.6. Let us emphasise the equivalence between Theorems 8.3.1 and 8.3.4 when Λ has dimension 0, *i.e.*, when it is the union of some discrete points. In this case, $T^*\Lambda = \{0\}\times\Lambda$ and the measure γ (that will not be on z) turns out to be

$$\gamma(\xi) = \sum_{\xi_0\in\Lambda}\alpha_{\xi_0}\delta(\xi-\xi_0), \quad \text{with} \quad \alpha_{\xi_0} = \|u_{\xi_0}(0,\cdot)\|^2_{L^2(\mathbb{R}^d)}.$$

In addition, $N^*_\xi\Lambda = \mathbb{R}^d$ and the operator $\mathfrak{M}(t,\xi)$ (which again does not depend on z) becomes the orthogonal projection onto $u_\xi(t,\cdot)$ in $L^2(\mathbb{R}^d)$, where, we recall, u_ξ solves the Schrödinger equation (8.3.4). Of course, these projections satisfy the Heisenberg equation (8.3.7).

8.4 The full effective mass equations

Theorems 8.3.1 and 8.3.4 fully describe the concentration of solutions to (8.3.1) – which has an interest in itself – and give effective mass equations for electrons in a crystalline lattice with initial states consisting of a sole Bloch mode.

It is not obvious that, for a superposition of the kind (8.2.6) that corresponds to electrons in general initial states, the result would be a sum over the particular measures linked to each mode, since neither the semiclassical measures nor the quadratic forms $|u^\varepsilon|^2$ are linear. Yet, under simple additional assumptions this is verified, what indicates that the interference terms between the different modes can be neglected in the semiclassical limit.

Basically, we will only need to impose that the Bloch energies have constant multiplicity and that the full initial state ψ^ε is ε-oscillating in a sense strictly stronger than usual. Thus, for every $n \in \mathbb{N}$ and $\Psi \in L^2(\mathbb{R}^d \times \mathbb{T}^d)$, define

$$P^\varepsilon_{\varphi_n}\Psi(x,y) = \varphi_n\left(\varepsilon\partial_x, y\right)\int_{\mathbb{T}^d}\varphi_n(\varepsilon\partial_x, z)^*\,\psi(x,z)\,dz \tag{8.4.1}$$

and, for every distinct Bloch eigenvalue λ_j, construct the Bloch spectral projector

$$\Pi^\varepsilon_{\lambda_j} = \sum_{P(\xi)\varphi_n(\xi,\cdot\,)=\lambda_j(\xi)\varphi_n(\xi,\cdot\,)} P^\varepsilon_{\varphi_n}. \tag{8.4.2}$$

Accordingly, denote by $I \subset \mathbb{N}$ the set of indices n such that the multiplicity of the Bloch energies $\lambda_n(\xi)$ as eigenvalues of $P(\xi)$ is constant for every $\xi \in \mathbb{R}^d$, so they do not cross; recall that this implies that λ_n are real analytic[110] for any $n \in I$. Hereafter, we will relabel these indices so as to have $1, 2, ..., n, ... \in I$ and

$$\lambda_1(\xi) < \lambda_2(\xi) < \cdots < \lambda_n(\xi) < \cdots \to \infty.$$

Observe that these inequalities and the fact that the Bloch energies are continuous and periodic imply that they are well separate, *i.e.*, given $j, l \in I$, $j \neq l$, then:

$$\inf_{\xi\in\mathbb{R}^d} |\lambda_j(\xi) - \lambda_l(\xi)| > 0. \tag{8.4.3}$$

The fundamental new hypothesis reads:

H0' For some $r > 2d$, the family of initial data $(\psi_0^\varepsilon)_{\varepsilon>0}$ is strongly ε-oscillating of order r:

$$\exists C > 0 \,:\, \forall\varepsilon > 0, \quad \|\left\langle\varepsilon\partial_x\right\rangle^r \psi_0^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant C,$$

and its energy is concentrated on the well separate Bloch eigenvalues:

$$\psi_0^\varepsilon(x) = \sum_{j\in I}\Pi^\varepsilon_{\lambda_j}\tilde{\psi}_0^\varepsilon\left(x, \frac{x}{\varepsilon}\right) + r^\varepsilon(x), \tag{8.4.4}$$

with $\|r^\varepsilon\|_{L^2(\mathbb{R}^d)} \longrightarrow 0$ as $\varepsilon \longrightarrow 0$.

Remark 8.4.1. See Remarks 10.2.1 and 10.2.18 for, respectively, an enlightening comment on the definition of strong ε-oscillation and its precise need in our analysis.

In what follows, we shall denote by $\Lambda_j \subset \mathbb{R}^d$ the set of critical points of the Bloch eigenvalue $\lambda_j(\xi)$ for $j \in \mathbb{N}$.

Theorem 8.4.2. *Assume* **H0'** *and* **H1** *and suppose that, for any $j \in I$,* **w-H2** *holds individually for the Bloch energies λ_j. Then there exists a sequence $(\varepsilon_k)_{k\in\mathbb{N}}$ tending to 0 and, for every $j \in I$, positive measures $\gamma_j \in \mathcal{M}(T^*\Lambda_j)$ and a measurable family of self-adjoint, positive, trace-class operators*

$$\mathfrak{M}_{0,j} : T^*\Lambda_j \ni (z,\xi) \longmapsto \mathfrak{M}_{0,j}(z,\xi) \in \mathcal{L}(L^2(N^*_\xi\Lambda_j)), \quad \operatorname{tr}_{L^2(N^*_\xi\Lambda_j)}\mathfrak{M}_{0,j}(z,\xi) = 1,$$

such that, for every $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, one has:

(8.4.5)
$$\lim_{k\to\infty}\int_{\mathbb{R}\times\mathbb{R}^d}\phi_t(x)|\psi^{\varepsilon_k}(t,x)|^2dxdt = \sum_{j\in I}\int_{\mathbb{R}\times T^*\Lambda_j}\operatorname{tr}_{L^2\left(N^*_\xi\Lambda_j\right)}\left(m_{\phi_t}(z,\xi)\,\mathfrak{M}_j(t,z,\xi)\right)\gamma_j(dz,d\xi)dt,$$

where the $C\left(\mathbb{R},\mathcal{L}\left(L^2(N^*_\xi\Lambda)\right)\right)$ functions $t \longmapsto \mathfrak{M}_j(t,z,\xi)$ solve the following Heisenberg equation with effective mass:

$$\text{(8.4.6)}\qquad \begin{cases} i\partial_t\,\mathfrak{M}_j(t,z,\xi) = \left[\,-\frac{1}{2}\nabla^2\lambda_j(\xi)\partial\cdot\partial + m_V(z,\xi)\,,\,\mathfrak{M}_j(t,z,\xi)\,\right] \\ \mathfrak{M}_j(0,z,\xi) = \mathfrak{M}_{0,j}(z,\xi). \end{cases}$$

Here, $M_{0,j} = \mathfrak{M}_{0,j}\gamma_j$ forms the operator-valued microlocal measure of the family $\left(\psi^{\varepsilon_k}_{0,j}\right)_{k\in\mathbb{N}}$ over Λ_j, where $\psi^\varepsilon_{0,j}(x) = \Pi^\varepsilon_{\lambda_j}\tilde{\psi}^\varepsilon_0\left(x,\frac{x}{\varepsilon}\right)$.

Re-writing Theorem 8.4.2 in the special case where the Bloch eigenvalues $\lambda_j(\xi)$ have a finite set of critical points:

Theorem 8.4.3. *Assume* **H0'**, **H1**, *and that* **s-H2** *holds for any Bloch eigenvalue λ_j, $j \in I$. Then there exists a sequence $(\varepsilon_k)_{k\in\mathbb{N}}$ tending to 0 such that, for every $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, the following holds:*

$$\text{(8.4.7)}\qquad \lim_{k\to\infty}\int_{\mathbb{R}\times\mathbb{R}^d}\phi(t,x)|\psi^{\varepsilon_k}(t,x)|^2dxdt = \sum_{j\in I}\sum_{\xi_0\in\Lambda_j}\int_{\mathbb{R}\times\mathbb{R}^d}\phi(t,x)|\psi_{\xi_0}(t,x)|^2dxdt,$$

where, for any $\xi_0 \in \Lambda_j$, ψ_{ξ_0} solves the Schrödinger equation with effective mass:

$$\text{(8.4.8)}\qquad \begin{cases} i\partial_t\psi_{\xi_0}(t,x) = -\frac{1}{2}\nabla^2\lambda_j(\xi_0)\partial_x\cdot\partial_x\,\psi_{\xi_0}(t,x) + V(x)\psi_{\xi_0}(t,x) \\ \psi_{\xi_0}(0,\cdot) = \operatorname{w}\lim\left(e^{-\frac{i}{\varepsilon_k}\xi_0\cdot x}\psi^{\varepsilon_k}_{0,j}\right), \end{cases}$$

this $L^2(\mathbb{R}^d)$ weak limit being unique, with $\psi^\varepsilon_{0,j}(x) = \Pi^\varepsilon_{\lambda_j}\tilde{\psi}^\varepsilon_0\left(x,\frac{x}{\varepsilon}\right)$.

As we can see, in Theorems 8.3.4 and 8.4.2 the time evolution of the weak limits of $|\psi^\varepsilon|^2$ is given by the natural Heisenberg dynamics of the microlocal measure with effective mass given by the Bloch energy, one only needing as an input some initial value for the measure. In the simplified cases stated in 8.3.1 and 8.4.3, the picture is even more favourable, for one can work directly with some weak limits of ψ^ε that obey to a Schrödinger equation with effective mass tensor given, again, by the Bloch energy.

In Chapter 11, we will perform some explicit calculations in order to analyse the different behaviours that can show up in cases where the Hessian $\nabla^2\lambda$ is or is not full rank. We hope that they will enlighten these theorems' applications, that are not as hard as they seem from their statements.

Chapter 9

Analysis of the Bloch modes

9.1 Localization over Λ

We will now consider Wigner distributions associated to solutions of the evolution equation:

$$i\varepsilon^2\partial_t u^\varepsilon(t,x) = \lambda(\varepsilon\partial_x)u^\varepsilon(t,x) + \varepsilon^2 V(x)u^\varepsilon(t,x) + \varepsilon^3 g^\varepsilon(t,x), \tag{9.1.1}$$

where V and λ satisfy hypothesis **H1** and $\|g^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)}$ is locally ε-uniformly bounded in t. We shall see in Chapter 10 that the analysis of the full Bloch decomposition reduces to analysing each of its modes satisfying an equation of the form (9.1.1).

It turns out that (9.1.1) is semiclassically very similar to equation (2.2.18) studied in the introductory Chapter 2: the terms $\varepsilon^2 V$ will produce terms of order ε^3 when commuted with pseudodifferential operators with smooth compactly supported symbols and $\varepsilon^3 g^\varepsilon$ will be negligible anyway, so we should expect to have the Wigner measures linked to the concentration of u^ε obeying to the same invariance properties we depicted in Section 2.2.3 for $b(x,\xi) = \lambda(\xi)$.

Indeed, the flow induced by this symbol on the phase space, $\Phi_s(x,\xi) = (x+s\nabla\lambda(\xi),\xi)$, leaves the semiclassical measures invariant, so they will not charge the regions where Φ is dispersive in the sense of Chapter 2, *i.e.*, where $\nabla\lambda(\xi) \neq 0$.

Let us re-state this fact and prove it directly:

Proposition 9.1.1. *Let be μ a semiclassical measure linked to a family $(u^\varepsilon)_{\varepsilon>0}$ of solutions to* (9.1.1) *and do $\mu = \mu_t dt$. Then, for almost every $t \in \mathbb{R}$, one has:*

$$\operatorname{supp}\mu_t \subset \Lambda = \{(x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d \ : \ \nabla\lambda(\xi) = 0\}.$$

Proof. In view of Lemma 2.2.6, it is sufficient to show that, for almost every $t \in \mathbb{R}$, the measure μ_t is invariant by $\Phi_s(x,\xi) = (x + s\nabla\lambda(\xi),\xi)$. This means that, for every Borelian function a on $\mathbb{R}^{2d}$ one has, for any $s \in \mathbb{R}$,

$$\int_{\mathbb{R}^{2d}} a \circ \Phi_s(x,\xi)\mu_t(dx,d\xi) = \int_{\mathbb{R}^{2d}} a(x,\xi)\mu_t(dx,d\xi).$$

It is enough to show that, for any $a \in C_0^\infty(\mathbb{R}^{2d})$ and $\Xi \in C_0^\infty(\mathbb{R})$,

$$\int_{\mathbb{R}\times\mathbb{R}^{2d}} \Xi(t)\left\langle \operatorname{op}_\varepsilon\left(\frac{d}{ds}a\circ\Phi_s(x,\xi)\bigg|_{s=0}\right)u_t^\varepsilon\,,\,u_t^\varepsilon\right\rangle dt \underset{\varepsilon\to 0}{\longrightarrow} 0 \tag{9.1.2}$$

(the reason why we only need to prove it at $s = 0$ is explained in the proof of Proposition 2.2.4).

Moreover, note that

$$\frac{d}{ds} a \circ \Phi_s(x,\xi)\Big|_{s=0} = \nabla_\xi \lambda(\xi) \cdot \nabla_x a(x,\xi) = \{\lambda(\xi)\,, a(x,\xi)\},$$

thus, from (2.1.4) we get

$$\operatorname{op}_\varepsilon\left(\frac{d}{ds}(a\circ\Phi_s)\Big|_{s=0}\right) = \frac{i}{\varepsilon}\left[\lambda(\varepsilon\partial_x)\,, \operatorname{op}_\varepsilon(a)\right] + \mathcal{O}_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)}(\varepsilon) \tag{9.1.3}$$

and, using the fact that u^ε solves (9.1.1):

$$\begin{aligned} \frac{i}{\varepsilon}\int_{\mathbb{R}} \Xi(t)\,\langle[\lambda(\varepsilon\partial_x)\,, \operatorname{op}_\varepsilon(a)]\,u_t^\varepsilon\,, u_t^\varepsilon\rangle\,dt &= -\varepsilon\int_{\mathbb{R}} \Xi(t)\frac{d}{dt}\langle \operatorname{op}_\varepsilon(a)u_t^\varepsilon\,, u_t^\varepsilon\rangle\,dt + \mathcal{O}(\varepsilon) \\ &= \varepsilon\int_{\mathbb{R}} \Xi'(t)\,\langle \operatorname{op}_\varepsilon(a)u_t^\varepsilon\,, u_t^\varepsilon\rangle\,dt + \mathcal{O}(\varepsilon) \\ &= \mathcal{O}(\varepsilon). \end{aligned} \tag{9.1.4}$$

This estimate and identity (9.1.3) show that (9.1.2) holds, hence the proposition. □

This fact is a restriction that the dynamics of u^ε imposes over the measures to which these functions may concentrate: in the region in the phase space where equation (9.1.1) is dispersive, the energy of a family $(u^\varepsilon)_{\varepsilon>0}$ solving (9.1.1) must vanish.

In addition, concentration on a submanifold of the phase space is a clue that one should analyse rather the two-microlocal measures instead of the Wigner ones; in particular, Proposition 9.1.1 does not explain how the measures μ_t depend on the sequence of initial data u_0^ε. Unlike in Part II, where this involved the semiclassical measures μ_0 of the sequence of initial data, that were then transported by some phase space flow, here this dependence is bounded to the underlying two-microlocal structure of the measures – in Example 11.1.2, Chapter 11, we will produce sequences of initial data having the same semiclassical measure, but such that their time dependent measures differ. This kind of behavior was first remarked in the case of the Schrödinger equation on the torus[77, 78].

Similar to what we have done in Part II are the guidelines to analyse the two-microlocal measures. Relying on Proposition 2.3.1 duly adapted, we will need to understand the geometric nature of the manifold Λ and choose a suitable set of coordinates wherein it coincide locally with a subspace of $\mathbb{R}^d$.

Thus, let us work out the two-microlocalization in our specific context by re-stating, *mutatis mutandis*, Proposition 2.3.1. First, redefine the symbol class $S(p)$ as composed by symbols $a \in C^\infty(\mathbb{R}^{2d+p})$ such that

- For each $\rho \in \mathbb{R}^p$, $(x,\xi) \longmapsto a(x,\xi,\rho)$ is compactly supported on $\mathbb{R}^{2d}_{x,\xi}$.
- There exists some $R_0 > 0$ and a function $a_\infty \in C^\infty(\mathbb{R}^{2d} \times \mathcal{S}^{p-1})$ such that, for $\|\rho\| > R_0$, one has $a(x,\xi,\rho) = a_\infty\left(x,\xi,\frac{\rho}{\|\rho\|}\right)$.

These symbols will be quantized as

$$\operatorname{op}_\varepsilon^\sharp(a(x,\xi,\rho)) = \operatorname{op}_\varepsilon\left(a\left(x,\xi,\frac{\xi''}{\varepsilon}\right)\right);$$

as before, the right-hand term above is just the banal quantization of a ε-dependent $\mathbb{R}^{2d}$ function as in (2.1.1).

Proposition 9.1.2. *There exists a measure ν on $\mathbb{R}\times\mathbb{R}^{2d-p}\times S^{p-1}$ and a trace class operator valued measure M on $\mathbb{R}\times\mathbb{R}^{2(d-p)}$, both positive, such that, for $a \in S(p)$ and $\Xi \in C_0^\infty(\mathbb{R})$,*

$$\begin{aligned} \operatorname{sc}\lim \int_{\mathbb{R}} \Xi(t)\,\langle\, \mathrm{op}_\varepsilon^\sharp(a)\Psi_t^\varepsilon\,,\,\Psi_t^\varepsilon\,\rangle\, dt &= \left\langle \mu(t,x,\xi)\mathbb{1}_{\{\xi''\neq 0\}}\,,\Xi(t)\,a_\infty\left(x,\xi,\frac{\xi''}{\|\xi''\|}\right)\right\rangle_{\mathbb{R}\times\mathbb{R}^{2d}} \\ &+ \ \langle\, \delta(\xi'')\otimes\nu(t,x,\xi',\omega)\,,\Xi(t)\,a_\infty\left(x,\xi,\omega\right)\rangle_{\mathbb{R}\times\mathbb{R}^{2d}\times S^{p+1}} \\ &+ \ \operatorname{tr}\langle\, M(t,x',\xi')\,,\,\Xi(t)\,a^w\left(x',y,\xi',0,\partial_y\right)\rangle_{\mathbb{R}\times\mathbb{R}^{2(d-p)}}\,, \end{aligned} \tag{9.1.5}$$

where $a^w(x',y,\xi',0,\partial_y)$ is the Weyl quantization of the symbol $(y,\zeta)\longmapsto a(x',y,\xi',0,\zeta)$ with $\varepsilon = 1$ and μ is the usual Wigner measure related to Ψ^ε.

The terms in (2.3.1) *are obtained respectively from those in the decomposition*

$$a(x,\xi,\rho) = a(x,\xi,\rho)\left(1-\chi\left(\frac{\xi''}{\delta}\right)\right) + a(x,\xi,\rho)\left(1-\chi\left(\frac{\rho}{R}\right)\right)\chi\left(\frac{\xi''}{\delta}\right) + a(x,\xi,\rho)\chi\left(\frac{\rho}{R}\right) \tag{9.1.6}$$

in the limit when $\varepsilon \longrightarrow 0$, then $R\longrightarrow\infty$, and last $\delta\longrightarrow 0$, where χ is a cut-off function such that $0\leqslant\chi\leqslant 1$, $\chi(\xi'') = 1$ for $\|\xi''\| < \frac{1}{2}$ and $\chi(\xi'') = 0$ for $\|\xi''\|\geqslant 1$.

Remark 9.1.3. A fact analogous to that exposed in Remark 2.3.2 is still valid. There, in the case where $p = d$, we had that for any compact operator T, $\operatorname{tr}(TM) = \langle T\Psi,\Psi\rangle$, with Ψ a weak limit of the family $(\Psi^\varepsilon)_{\varepsilon>0}$ linked to the measure M. Here one should replace Ψ by its Fourier transform $\hat{\Psi}$. It is this simplification that allows Theorems 8.3.4 and 8.4.2 to have their short versions 8.3.1 and 8.4.3.

Remark 9.1.4. Since M is absolutely continuous with respect to the Lebesgue measure dt[1], one has $M = M_t dt$, where each M_t is an operator-valued measure. Moreover, the Radon-Nikodym theorem allows us to decompose these M_t as an operator-valued function $\mathfrak{M}(t,\cdot\,)$ and scalar measures γ_t, whence $M_t(x',\xi') = \mathfrak{M}(t,x',\xi')\gamma_t(x',\xi')dt$. We will see in Proposition 9.4.8 that the dependence on t can be conveniently stripped off from the measure part γ. Last, remark that this decomposition is not unique, since given any $C>0$, the pair $C\,\mathfrak{M}$ and $\frac{1}{C}\gamma$ also works.

9.2 The case $\dim\Lambda = 0$

In this section we will prove Theorem 8.3.1. Even though it is a particular case of 8.3.4, its proof is far simpler and enlightens the way one obtains discrete results in microlocal analysis.

Supposing **H1** and **s-H2**, Λ is a finite set of isolated critical points of λ. Letting μ be the semiclassical measure linked to the family $(u^\varepsilon)_{\varepsilon>0}$ through some subsequence, Proposition 9.1.1 gives

$$\mu = \sum_{\xi_0\in\Lambda} \mu\mathbb{1}_{\{\xi=\xi_0\}}, \tag{9.2.1}$$

so we basically need to microlocalize the Wigner measure over each affine space $\{\xi=\xi_0\}$ and study the corresponding measures ν_{ξ_0} and M_{ξ_0}. Strictly speaking, we should perform a variable change that consists of a translation $\xi\longmapsto\zeta+\xi_0$ so that these spaces become vectorial, $\{\zeta = 0\}$, but if we simply redefine

$$\mathrm{op}_\varepsilon^\sharp(a(x,\xi,\rho)) = \mathrm{op}_\varepsilon\left(a\left(x,\xi,\frac{\xi-\xi_0}{\varepsilon}\right)\right),$$

[1]For so are the Wigner measures μ, what extends to the two-microlocal measures ν_∞ and M by positivity.

then the effect is exactly the same and decomposition (9.1.6) will give the microlocal measures ν_{ξ_0} and M_{ξ_0} that we want in the limits $\varepsilon \longrightarrow 0$, $R \longrightarrow \infty$ and $\delta \longrightarrow 0$.

Below, we present some results about the two-microlocal measures for u^ε solving equation (9.1.1).

Lemma 9.2.1. *Write $M_{\xi_0}(t) = \mathfrak{M}_{\xi_o}(t)dt$. Then the function $\mathbb{R} \ni t \longmapsto \mathfrak{M}_{\xi_0}(t)$ into the trace class operators equipped with the weak topology is continuous.*

Proof. From the Ascoli-Arzelà theorem, it is sufficient to prove that

$$\mathbb{R} \ni t \longmapsto I^{\varepsilon,R}(t) = \left\langle \mathrm{op}_\varepsilon^\sharp \left(a(x,\xi,\rho)\chi\left(\frac{\rho}{R}\right)\right) u_t^\varepsilon \, , u_t^\varepsilon \right\rangle \in \mathbb{R}$$

is equibounded and equicontinuous with respect to ε and R. Equiboundedness is obvious from (2.1.2) and the boundedness of the family u^ε uniformly in ε; for equicontinuity, observe that

$$I^{\varepsilon,R}(t) = \langle \mathrm{op}_1 \left(a_R^\varepsilon\right) v_t^\varepsilon \, , v_t^\varepsilon \rangle \,, \tag{9.2.2}$$

where

$$a_R^\varepsilon(x,\xi) = a\left(x,\xi_0 + \varepsilon\xi,\xi\right)\chi\left(\frac{\xi}{R}\right) \quad \text{and} \quad v^\varepsilon(t,x) = e^{-\frac{i}{\varepsilon}\xi_0 \cdot x} u^\varepsilon(t,x);$$

since u^ε solves (9.1.1), passing to the momentum space one sees that $\hat{v}^\varepsilon$ satisfies

$$\begin{aligned} i\varepsilon^2\partial_t \hat{v}^\varepsilon(t,\xi) &= \lambda(\xi_0+\varepsilon\xi)\hat{v}^\varepsilon(t,\xi) + \varepsilon^2 V(-\partial_\xi)\hat{v}^\varepsilon(t,\xi) + \mathcal{O}_{L^2(\mathbb{R}^d)}\left(\varepsilon^3\right) \\ &= \lambda(\xi_0)\hat{v}^\varepsilon(t,\xi) + \frac{\varepsilon^2}{2}\nabla^2\lambda(\xi_0)\xi^{(2)}\hat{v}^\varepsilon(t,\xi) + \varepsilon^2 V(-\partial_\xi)\hat{v}^\varepsilon(t,\xi) + \mathcal{O}_{L^2(\mathbb{R}^d)}\left(\varepsilon^3\right), \end{aligned} \tag{9.2.3}$$

where we used that $\xi_0 \in \Lambda$, so $\nabla\lambda(\xi_0) = 0$. Thus, setting $\hat{u}^\varepsilon_{\xi_0}(t,\cdot) = e^{-\frac{it}{\varepsilon^2}\lambda(\xi_0)}\hat{v}^\varepsilon(t,\cdot)$ and passing back to the position space, this newly defined function obeys to

$$i\partial_t u^\varepsilon_{\xi_0}(t,x) = -\frac{1}{2}\nabla^2\lambda(\xi_0)\partial_x \cdot \partial_x u^\varepsilon_{\xi_0}(t,x) + V(x)u^\varepsilon_{\xi_0}(t,x) + \mathcal{O}_{L^2(\mathbb{R}^d)}\left(\varepsilon\right) \tag{9.2.4}$$

with initial datum $u^\varepsilon_{\xi_0}(0,x) = v^\varepsilon(0,x)$.

Of course, adding to the functions v_t^ε a phase that is constant in x does not change in anything the inner product in (9.2.2), so one gets:

$$\begin{aligned} I^{\varepsilon,R}(t) &= \left\langle \mathrm{op}_1\left(a_R^\varepsilon\right) u^\varepsilon_{\xi_0,t} \, , u^\varepsilon_{\xi_0,t}\right\rangle \\ &= \left\langle \mathrm{op}_\varepsilon \left(a\left(x,\xi_0+\xi,\frac{\xi}{\varepsilon}\right)\chi\left(\frac{\xi}{\varepsilon R}\right)\right) u^\varepsilon_{\xi_0,t} \, , u^\varepsilon_{\xi_0,t}\right\rangle . \end{aligned} \tag{9.2.5}$$

Taking the derivative with respect to t, doing standard symbolic calculus and considering that $u^\varepsilon_{\xi_0,t}$ are also uniformly bounded with respect to ε and R:

$$\begin{aligned} \frac{d}{dt}I^{\varepsilon,R}(t) &= \left\langle i\left[-\frac{1}{2}\nabla^2\lambda(\xi_0)\partial_x \cdot \partial_x + V(x) \, , \mathrm{op}_\varepsilon\left(a\left(x,\xi_0+\xi,\frac{\xi}{\varepsilon}\right)\chi\left(\frac{\xi}{\varepsilon R}\right)\right)\right] u^\varepsilon_{\xi_0,t} \, , u^\varepsilon_{\xi_0,t}\right\rangle \\ &= \varepsilon\left\langle \mathrm{op}_\varepsilon\left(\left\{\frac{1}{2}\nabla^2\lambda(\xi_0)\xi^2 + V(x) \, , a\left(x,\xi_0+\xi,\frac{\xi}{\varepsilon}\right)\chi\left(\frac{\xi}{\varepsilon R}\right)\right\}\right) u^\varepsilon_{\xi_0,t} \, , u^\varepsilon_{\xi_0,t}\right\rangle + \mathcal{O}\left(1+\varepsilon^2+\frac{1}{R^2}\right) \\ &= \mathcal{O}\left(1+\varepsilon+\frac{1}{R}\right); \end{aligned}$$

equiboundedness now follows from a trivial application of the mean value theorem.

As a conclusion, given any compact K, the limits of $K \ni t \longmapsto I^{\varepsilon,R}(t) \in \mathbb{R}$ will be continuous and so will be $\mathbb{R} \ni t \longmapsto \mathfrak{M}_{\xi_0}(t)$ into the trace class operators with weak topology, since the trace of $\mathfrak{M}_{\xi_0}$ against any compact operator will be tested against functions compactly supported in time. ◻

Lemma 9.2.2. $\mathfrak{M}_{\xi_0}(t) = |u_{\xi_0}(t,\cdot)\rangle\,\langle u_{\xi_0}(t,\cdot)|$, *where* u_{ξ_0} *solves*

$$\begin{cases} i\partial_t u_{\xi_0}(t,x) = -\frac{1}{2}\nabla^2\lambda(\xi_0)\partial_x \cdot \partial_x\, u_{\xi_0}(t,x) + V(x)u_{\xi_0}(t,x) \\ u_{\xi_0}(0,\cdot) = \mathrm{w}\lim\left(e^{-\frac{i}{\varepsilon}\xi_0\cdot x}u_0^\varepsilon\right). \end{cases} \tag{9.2.6}$$

Proof. Let us start from the first line in (9.2.5) and calculate:

$$\left\langle \mathrm{op}_1\left(a_R^\varepsilon\right) u_{\xi_0,t}^\varepsilon\,, u_{\xi_0,t}^\varepsilon\right\rangle = \left\langle \mathrm{op}_1\left(a_R^0\right) u_{\xi_0,t}^\varepsilon\,, u_{\xi_0,t}^\varepsilon\right\rangle + R^\varepsilon,$$

where $\mathrm{op}_1(a_R^0)$ is the Weyl quantization of the symbol $(y,\zeta) \longmapsto a(y,\xi_0,\zeta)\chi\left(\frac{\zeta}{R}\right)$, and where

$$R^\varepsilon = \varepsilon\int_{\mathbb{R}^{3d}}\int_0^1 \frac{e^{i\xi\cdot(x-y)}}{(2\pi)^d}\nabla_\xi a\left(\frac{x+y}{2},\xi_0+\varepsilon s\xi,\xi\right)\cdot\xi\,\chi\left(\frac{\xi}{R}\right)v_t^\varepsilon(y)\overline{v_t^\varepsilon(x)}dsd\xi dydx$$

is of course an error of order ε for each fixed R, what makes that both inner products above coincide in the semiclassical limit.

Again, for each fixed R, a_R^0 is compactly supported and $\mathrm{op}_1(a_R^0)$ is a compact operator, hence, choosing a sequence ε_k going to 0 in such a manner that $u_{\xi_0,t}^{\varepsilon_k}$ converges weakly in $L^2(\mathbb{R}^d)$ to some $u_{\xi_0,t}$ for all t in a dense countable set $\Upsilon \subset \mathbb{R}$ containing 0[2], we obtain:

$$\left\langle \mathrm{op}_\varepsilon^\sharp\left(a(x,\xi,\rho)\chi\left(\frac{\rho}{R}\right)\right)u_t^\varepsilon\,, u_t^\varepsilon\right\rangle \longrightarrow \left\langle \mathrm{op}_1\left(a_R^0\right)u_{\xi_0,t}\,, u_{\xi_0,t}\right\rangle \quad \text{for } t\in\Upsilon; \tag{9.2.7}$$

From Lemma 9.2.1, given a compact $K \subset \mathbb{R}$, we can extend (9.2.7) to the whole closure $K = \overline{K\cap\Upsilon}$ by continuity. As a result, for any $\Xi \in C_0^\infty(\mathbb{R})$:

$$\int_{\mathbb{R}}\Xi(t)\left\langle \mathrm{op}_\varepsilon^\sharp\left(a(x,\xi,\rho)\chi\left(\frac{\rho}{R}\right)\right)u_t^\varepsilon\,, u_t^\varepsilon\right\rangle dt \longrightarrow \int_{\mathbb{R}}\Xi(t)\left\langle \mathrm{op}_1\left(a_R^0\right)u_{\xi_0,t}\,, u_{\xi_0,t}\right\rangle dt,$$

where it is clear that u_{ξ_0} satisfies the differential equation in the lemma's statement as a consequence of equation (9.2.4) and of $\varepsilon \longrightarrow 0$. Its initial datum comes from the very same weak limit since we supposed that $0\in\Upsilon$, justifying Remark 8.3.2.

Finally, remark that the inner product in the right-hand side of the expression above reads

$$\left\langle \mathrm{op}_1\left(a_R^0\right)u_{\xi_0,t}\,, u_{\xi_0,t}\right\rangle = \int_{\mathbb{R}^{2d}} kA_R(x,y)kU_{\xi_0,t}(y,x)dydx, \tag{9.2.8}$$

where kA_R is the integral kernel of $\mathrm{op}_1\left(a_R^0\right)$, and $kU_{\xi_0,t}$ of the operator

$$U_{\xi_0,t} = |u_{\xi_0}(t,\cdot)\rangle\,\langle u_{\xi_0}(t,\cdot)|\,.$$

The result then follows by letting R go to ∞. □

Lemma 9.2.3. *Measure* ν_{ξ_0} *is invariant by the flow*

$$\Phi_s : \mathbb{R}^d\times\mathcal{S}^{d-1} \ni (x,\omega) \longmapsto \left(x + s\,\nabla^2\lambda(\xi_0)\omega\,,\omega\right) \in \mathbb{R}^d\times\mathcal{S}^{d-1}.$$

[2]Such a sequence may be obtained though a process of Cantor diagonal extraction from the countable sequences $\varepsilon_k(t)$ that make $u_{\xi_0,t}^{\varepsilon_k(t)}$ converge to $u_{\xi_0,t}$ for each t in Υ.

Proof. This proof follows the lines of Proposition's 9.1.1 one. To begin with, let us set

$$\tilde{\Phi}_s(x,\xi,\rho) = \left(x + s\nabla^2\lambda_j(\xi_0)\rho\,,\xi,\rho\right), \quad (x,\xi,\rho)\in\mathbb{R}^d\times\mathbb{R}^d\times\mathbb{R}^d,$$

and

$$a_{R,\delta}(x,\xi,\rho) = a(x,\xi,\rho)\chi\left(\frac{\xi-\xi_0}{\delta}\right)\left(1-\chi\left(\frac{\rho}{R}\right)\right).$$

Using a Taylor expansion and the fact that $\xi_0\in\Lambda$, one has

$$\nabla\lambda(\xi) = \nabla^2\lambda(\xi_0)(\xi-\xi_0) + \Gamma(\xi)(\xi-\xi_0)^{(2)},$$

where Γ is a smooth bounded tensor of order 3. Consequently, noticing that

$$\frac{d}{ds}\,a_{R,\delta}\circ\tilde{\Phi}_s(x,\xi,\rho)\Big|_{s=0} = \nabla_x\,a_{R,\delta}(x,\xi,\rho)\,\centerdot\,\nabla^2\lambda(\xi_0)(\xi-\xi_0),$$

it follows that

$$\frac{d}{ds}\,a_{R,\delta}\circ\tilde{\Phi}_s(x,\xi,\rho)\Big|_{s=0} = \nabla_\xi\lambda(\xi)\,\centerdot\,\nabla_x\,a_{R,\delta}(x,\xi,\rho) + \Gamma(\xi)(\xi-\xi_0)^{(2)}\,\centerdot\,\nabla_x\,a_{R,\delta}(x,\xi,\rho).$$

By standard symbolic calculus, we have either

$$\mathrm{op}_\varepsilon^\sharp\left(\Gamma(\xi)(\xi-\xi_0)^{(2)}\,\centerdot\,\nabla_x\,a_{R,\delta}\right) = \mathcal{O}\left(\varepsilon^2\right)$$

and

$$\begin{aligned}\mathrm{op}_\varepsilon^\sharp\left(\nabla_\xi\lambda\,\centerdot\,\nabla_x\,a_{R,\delta}\right) &= \frac{i}{\varepsilon}\left[\lambda(\varepsilon\partial_x)\,,\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\right)\right] + \mathcal{O}(\varepsilon/\delta) + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}(\delta)\\ &= \frac{i}{\varepsilon}\left[\lambda(\varepsilon\partial_x) + \varepsilon^2 V(x)\,,\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\right)\right] + \mathcal{O}\left(\varepsilon\right) + \mathcal{O}\left(\frac{\varepsilon}{\delta}\right) + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}(\delta),\end{aligned}$$

where all the errors are meant to be in $\mathcal{L}\left(L^2(\mathbb{R}^d)\right)$. Therefore,

$$\begin{aligned}&\int_{\mathbb{R}}\Xi(t)\left\langle\mathrm{op}_\varepsilon^\sharp\left(\frac{d}{ds}\,a_{R,\delta}\circ\tilde{\Phi}_s\Big|_{s=0}\right)u_t^\varepsilon\,,u_t^\varepsilon\right\rangle dt\\ &\quad= \varepsilon\int_{\mathbb{R}}\Xi(t)\frac{d}{dt}\left\langle\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\right)u_t^\varepsilon\,,u_t^\varepsilon\right\rangle dt + \mathcal{O}\left(\varepsilon\right) + \mathcal{O}\left(\frac{\varepsilon}{\delta}\right) + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left(\delta\right)\\ &\quad= -\varepsilon\int_{\mathbb{R}}\Xi'(t)\left\langle\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\right)u_t^\varepsilon\,,u_t^\varepsilon\right\rangle dt + \mathcal{O}\left(\varepsilon\right) + \mathcal{O}\left(\frac{\varepsilon}{\delta}\right) + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left(\delta\right)\\ &\quad= \mathcal{O}\left(\varepsilon\right) + \mathcal{O}\left(\frac{\varepsilon}{\delta}\right) + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left(\delta\right),\end{aligned}$$

thus, letting ε go to 0, then R to ∞ and last δ to 0, we obtain:

$$\int_{\mathbb{R}\times\mathbb{R}^d\times\mathcal{S}^{d-1}}\Xi(t)\,\frac{d}{ds}\tilde{a}_\infty\circ\Phi_s(x,\omega)\Big|_{s=0}\nu_{\xi_0}(dt,dx,d\omega) = 0,$$

with $\tilde{a}_\infty(x,\omega) = a_\infty(x,\xi_0,\omega)$. Since this relation holds for any Ξ in $C_0^\infty(\mathbb{R})$ and $a\in S(d)$, ν_{ξ_0} is invariant by Φ. □

Bringing together Lemmata 9.2.2, 9.2.3 and the fact Φ in this last lemma is dispersive for $\nabla^2\lambda(\xi_0)$ non-degenerate:

Proposition 9.2.4. *If **H1** and **s-H2** hold, then one has*

$$\mu(t,x,\xi) = \sum_{\xi_0\in\Lambda} |u_{\xi_0}(t,x)|^2\, \delta(\xi-\xi_0)\otimes dx\otimes dt,$$

with u_{ξ_0} being given in Lemma 9.2.2.

Proof. Considering **s-H2**, the flow through which ν_{ξ_0} is invariant in Lemma 9.2.3 is dispersive, thus from Lemma 2.2.6 one has $\nu_{\xi_0} = 0$ and the only term in the microlocal decomposition of $\mu \mathbb{1}_{\{\xi=\xi_0\}}$ is that with M_{ξ_0}. This measure is explicitly given in Lemma 9.2.2, and a simple calculation shows that, when $a \in C_0^\infty(\mathbb{R}^{2d})$ (*i.e.*, $a \in S(d)$ is constant on ρ), equation (9.2.8) gives by dominated convergence:

$$\begin{aligned}\lim_{R\to\infty} \left\langle \mathrm{op}_1\left(a_R^0\right) u_{\xi_0,t}\,, u_{\xi_0,t}\right\rangle &= \int_{\mathbb{R}^{3d}} \frac{e^{i\xi\cdot(x-y)}}{(2\pi)^d} a\left(\frac{x+y}{2},\xi_0\right) u_{\xi_0}(t,y)\overline{u_{\xi_0}(t,x)}d\xi dy dx\\ &= \int_{\mathbb{R}^d} a(x,\xi_0)\,|u_{\xi_0}(t,x)|^2\,dx.\end{aligned}$$

From equation (9.2.1), one knows that the full Wigner measure μ is just the sum of these terms for $\xi_0\in\Lambda$. □

This proposition gives Theorem 8.3.1 directly when integrating the Wigner measure μ with respect to ξ under hypothesis **H0** of ε-oscillation.

9.3 The geometry of Λ

Let us now switch **s-H2** and **w-H2**, so Λ ceases to be a discrete set and becomes a continuum. As in Part II, we need to look for a new system of coordinates wherein Λ have so simple an algebraic expression as $\xi''=0$, which makes the analysis of the two-microlocal measures feasible according to Proposition 9.1.2.

In order to do so, hereafter we shall look at Λ intrinsically, separating its points from their natural Cartesian coordinates in $\mathbb{R}^d$.

9.3.1 Geodesic coordinates

In each point $\sigma\in\Lambda$, there exists an orthonormal set of vectors $\left\{\mathbf{n}_\sigma^1,\dots,\mathbf{n}_\sigma^p\right\}\subset\mathbb{R}^d$ forming a basis of $N_\sigma\Lambda$, and there exists a tubular neighbourhood $\Omega\subset\mathbb{R}^d$ of Λ where one can define normal geodesic coordinates: to any $\theta\in\Omega$, one associates unique $\sigma(\theta)\in\Lambda\subset\mathbb{R}^d$ and $\rho(\theta)\in\mathbb{R}^p$ such that

$$\theta = \sigma(\theta) + \mathrm{Exp}_{\sigma(\theta)}\left[\rho(\theta)\right], \tag{9.3.1}$$

where $\mathrm{Exp}_\sigma(\rho)$ denotes the point at time $\|\rho\|$ in the geodesic trajectory arising from σ in the direction $\sum_{j=1}^p \frac{\rho_j}{\|\rho\|}\mathbf{n}_\sigma^j$.

Naturally, Ω has its straightforward Cartesian coordinates denoted by ξ, in which the local expression of θ is trivially $\xi_\theta=\theta$. Nevertheless, given an atlas $\mathbb{A}'$ for Λ with local charts κ',

$$\kappa'\;:\;V\cap\Lambda\longrightarrow U'\subset\mathbb{R}^{d-p},$$

where V are open sets of $\mathbb{R}^d$ and U' of $\mathbb{R}^{d-p}$, we can build more interesting local coordinate systems in $V \cap \Omega$, that we denote by κ and which are given by

$$\begin{array}{rcccc} \kappa & : & V \cap \Omega & \longrightarrow & U \times \mathbb{R}^p \\ & & \theta & \longmapsto & \zeta_\theta = \begin{pmatrix} \kappa'(\sigma(\theta)) \\ \rho(\theta) \end{pmatrix}, \end{array} \tag{9.3.2}$$

$U \subset \mathbb{R}^{d-p}$ open containing U', and result in a new atlas $\mathbb{A}$ for Ω.

Let us denote by ζ_θ the local expression for θ in this new atlas; observe that now $\zeta_\theta \neq \theta$. For convenience, we will write $\zeta = (\zeta', \zeta'')$, with $\zeta' \in \mathbb{R}^{d-p}$ and $\zeta'' \in \mathbb{R}^p$, so as in this new system of coordinates the sets $\kappa(V \cap \Lambda)$ are given just by the equation $\zeta'' = 0$, *regardless the particular local charts* κ chosen on Ω.

Remark 9.3.1. Being a $\mathbb{R}^d$ neighbourhood of Λ, Ω is itself a d-dimensional submanifold of $\mathbb{R}^d$ with its natural Cartesian coordinates. Thus, equipping it with a new coordinate system is equivalent to saying that it is diffeormorphic to another submanifold Ω_0, which is nothing else than the pair $(\Omega, \mathbb{A})$. This same diffeomorphism maps the submanifold $\Lambda = \{\sigma \in \Omega,\ \nabla\lambda(\xi_\sigma) = 0\}$ to $\Lambda_0 = \{\sigma \in \Omega_0,\ \zeta''_\sigma = 0\}$: if κ is a local chart of Ω, then its projection $\pi\kappa$, with $\pi = [\,\mathbb{1}_{d-p\times d-p}\ \ \mathbf{0}_{d-p\times p}\,]$, serves as a chart for Λ when restricted to it, and we can call Λ_0 the pair formed by Λ and the atlas given by the projections $\pi\kappa$.

It happens that $\pi\kappa|_\Lambda = \kappa'$, so we are reduced to have Λ_0 and Λ coincide even in the sense of manifolds, *i.e.*, they are the same sets provided with the same local charts. Nonetheless, we will keep the notation Λ_0 for the pair $(\Lambda, \mathbb{A}')$, while Λ will be used to denote simply the set of singularities of λ, whose points will be expressed in the original $\mathbb{R}^d$ coordinates with no risk of misunderstanding, even though those could not properly be coordinates of a $d-p$ dimensional manifold.

This precious way of describing the coordinate changes will turn out to be helpful in Remarks 9.3.2 and 9.3.3.

Henceforth we will work in Ω_0 and study the concentration of the Wigner measure over Λ_0, where we are allowed to use the two-microlocal measures as in Proposition 9.1.2. Once we have the description we want, we will pull these measures back to the original coordinates, *i.e.*, to Λ.

Three issues arise, though. To decompose the phase space region Ω_0 as the direct sum of some tangent and normal bundles of Λ_0; to describe the coordinate transformations taking place when one changes between different charts $\kappa_1, \kappa_2 \in \mathbb{A}$ of Ω_0; and to obtain an analogous of Corollary 4.1.3 allowing us to transpose our microlocal objects ν and M from Λ_0 onto Λ, which consists of recognising how their explicit forms in coordinates should change.

9.3.2 Some bundles over Λ

To begin with, observe that, if $\kappa_1, \kappa_2 \in \mathbb{A}$ are such that $V_1 \cap V_2 \cap \Omega_0 \neq \emptyset$, their transition function $\vartheta = \kappa_1 \circ \kappa_2^{-1}$ will be a local diffeomorphism having the form

$$\zeta = \begin{pmatrix} \zeta' \\ \zeta'' \end{pmatrix} \longmapsto \begin{pmatrix} \vartheta'(\zeta') \\ \zeta'' \end{pmatrix} = \vartheta(\zeta), \tag{9.3.3}$$

where ϑ' is a local diffeomorphism of $\mathbb{R}^{d-p}$ that coincides with the transition function between κ'_1 and κ'_2 in Λ_0, $\vartheta' = \kappa'_1 \circ {\kappa'}_2^{-1}$. This means that any coordinate change in Ω_0

automatically induces one in Λ_0 and conversely. Its differential is:

$$\nabla\vartheta = \begin{bmatrix} \nabla_{\zeta'}\vartheta' & \mathbf{0} \\ \mathbf{0} & \mathbb{1}_{p\times p} \end{bmatrix}.$$

The cotangent transformation induced on $T^*\Omega_0$ by the coordinate change ϑ reads

$$\tilde{\vartheta} \ : \ \begin{array}{ccc} (z,\zeta) & \longmapsto & \left({}^t\nabla\vartheta(\zeta)^{-1}z, \vartheta(\zeta)\right) \\ (z',z'',\zeta',\zeta'') & \longmapsto & \left({}^t\nabla_{\zeta'}\vartheta'(\zeta')^{-1}z', z'', \vartheta'(\zeta'), \zeta''\right) \end{array} \tag{9.3.4}$$

and preserves the cotangent bundle $T^*\Lambda_0$, inducing there a similar change in local coordinates,

$$\vartheta_{T^*} : (z',\zeta') \longmapsto \left({}^t\nabla_{\zeta'}\vartheta'(\zeta')^{-1}z', \vartheta'(\zeta')\right), \tag{9.3.5}$$

and allowing us to consider $T^*_\sigma\Lambda_0$ as an invariant subspace of $T^*_\sigma\Omega_0$, $T^*_\sigma\Lambda_0 = \pi\left(T^*_\sigma\Omega_0\right)$, with π the projection on the first $d-p$ components, as in Remark 9.3.1.

Defining the conormal bundle $N^*\Lambda_0$ as having fibres

$$N^*_\sigma\Lambda_0 = {T^*_\sigma\Omega_0}\big/{T^*_\sigma\Lambda_0},$$

one sees that each fibre is also invariant by $\tilde{\vartheta}$: denoting $\pi^\perp = [\,\mathbf{0}_{p\times d-p}\ \ \mathbb{1}_{p\times p}\,]$, one has $N^*_\sigma\Lambda_0 = \pi^\perp\left(T^*_\sigma\Omega_0\right)$, and the coordinate change induced by ϑ is simply the identity in z'':

$$\vartheta_{N^*} : (z'',\zeta') \longmapsto (z'', \vartheta'(\zeta')). \tag{9.3.6}$$

Remark 9.3.2. For what concerns Λ, we still have $T^*_\sigma\Lambda \subset T^*_\sigma\Omega$, and the elements of $T^*_\sigma\Omega$ can be fairly given their original Cartesian coordinates as the $\mathbb{R}^d$ vectors they are; so, in the spirit of Remark 9.3.1, we shall denote the elements of $T^*_\sigma\Lambda$ by these same coordinates, even though they will not be proper coordinates in the sense of manifolds, as we have seen. Moreover, one may not have $T^*_\sigma\Lambda = \pi(T^*_\sigma\Omega)$ for π independent of σ like above, which means that we cannot just pick up the first $d-p$ coordinates of the elements of $T^*_\sigma\Omega$ and pretend that they mean something for the elements of $T^*_\sigma\Lambda$.

Yet, an element v_σ of $T^*_\sigma\Lambda$ is an element of $\mathbb{R}^d$ and, as such, it has Cartesian coordinates x_{v_σ}. As for $\theta \in \Omega$ we had $\xi_\theta = \theta$, here v_σ also coincides with its "coordinates", so we trivially have $x_{v_\sigma} = v_\sigma$. From the geometric relations between $T^*_\sigma\Omega_0$ and $T^*_\sigma\Omega$, it is clear that

$$(z'_{v_\sigma}, 0) = {}^t\nabla\kappa(\xi_\sigma)^{-1}x_{v_\sigma}, \tag{9.3.7}$$

which gives a one-to-one correspondence between the new (and genuine) coordinates z'_{v_σ} and the old x_{v_σ}.

The same considerations hold for the conormal space. Besides, now we also have $N^*_\sigma\Lambda = \operatorname{span}\left\{\mathbf{n}^1_\sigma, \dots, \mathbf{n}^p_\sigma\right\}$, thus, taking an element $w_\sigma \in N^*_\sigma\Lambda$ with $\mathbb{R}^d$ coordinates $x_{w_\sigma} = \left(x^1_{w_\sigma}, \dots, x^d_{w_\sigma}\right)$, we have $x_{w_\sigma} = \sum_{j=1}^p x^j_{w_\sigma}\mathbf{n}^j_\sigma$ and, further,

$$(0, z''_{w_\sigma}) = {}^t\nabla\kappa(\xi_\sigma)^{-1}x_{w_\sigma}, \tag{9.3.8}$$

which gives a one-to-one correspondence between z''_{w_σ} and x_{w_σ}.

Remark 9.3.3. Therefore, considering the decomposition

$$T^*_\sigma\Omega = T^*_\sigma\Lambda \oplus N^*_\sigma\Lambda,$$

we can take any $\varpi \in T^*_\sigma\Omega_0$ and write $\varpi = v_\sigma + w_\sigma$, where $v_\sigma \in T^*_\sigma\Lambda_0$ has coordinates z' and $w_\sigma \in N^*_\sigma\Lambda_0$ has z''; the local coordinates of ϖ will be $z = (z', z'')$. Consequently, going to $T^*_\sigma\Omega$, one can decompose any element x of $\mathbb{R}^d$ (at least in the neighbourhood Ω of Λ where $x =^t \nabla\kappa \circ \kappa^{-1}(\zeta)z$) as

$$x = x^{T^*} + x^{N^*},$$

where, in view of Remark 9.3.2, x^T depends bijectively on z', and x^N on z''; additionally $x^N \in \operatorname{span}\left\{\mathbf{n}^1_\sigma, \dots, \mathbf{n}^p_\sigma\right\}$ and $x^T \perp x^N$.

Resuming the analysis of the bundles over Λ_0, we associate to $N^*_\sigma\Lambda_0$ its dual space $N_\sigma\Lambda_0 = (N^*_\sigma\Lambda_0)^*$, defining then the standard normal bundle $N\Lambda_0$ above Λ_0. For the sake of notation, we will denote its elements by ζ''. Finally, taking the quotient of $N_\sigma\Lambda_0$ by dilatations:

$$S_\sigma\Lambda_0 = {N_\sigma\Lambda_0}/{\mathbb{R}^*_+},$$

we define the normal bundle in sphere, $S\Lambda_0$. Similarly to $N^*\Lambda_0$, the local expressions for these bundles' elements are transformed in a simple way:

$$\begin{array}{lclcl} \vartheta_N & : & (\zeta', \zeta'') & \longmapsto & (\vartheta'(\zeta'), \zeta''), \\ \vartheta_S & : & (\zeta', \omega) & \longmapsto & (\vartheta'(\zeta'), \omega). \end{array} \tag{9.3.9}$$

Putting this all together, we define an extended bundle $E\Lambda_0$ with fibres

$$E_\sigma\Lambda_0 = T^*_\sigma\Lambda_0 \oplus N^*_\sigma\Lambda_0 \oplus N_\sigma\Lambda_0. \tag{9.3.10}$$

$E\Lambda_0$ transforms exactly like $T^*\Omega_0$ in equation (9.3.4), so it is roughly a reconstruction of the phase space around the singularities, $T^*_{\Lambda_0}\Omega_0$, based exclusively on the structure of the submanifold Λ_0.

Another definition that we will need is the extended bundle in sphere $SE\Lambda_0$, with fibres

$$SE_\sigma\Lambda_0 = T^*_\sigma\Lambda_0 \oplus N^*_\sigma\Lambda_0 \oplus S_\sigma\Lambda_0. \tag{9.3.11}$$

Both bundles transform using in each fibre the functions ϑ_{T^*}, ϑ_{N^*} and ϑ_N or ϑ_S presented in (9.3.5), (9.3.6) and (9.3.9) respectively. Let us call their transformations κ_E and κ_{SE}.

In Part II, we saw in Corollary 4.1.3 that ν_∞ and $\mathfrak{m}$ were measures on $\mathbb{R} \times SE\Lambda$ and $\mathbb{R} \times E\Lambda$ respectively. Here we will also need to use the operator-valued measure M, so let us define a new functional bundle $\mathcal{H}\Lambda$, having fibres:

$$\mathcal{H}_\sigma\Lambda = \mathcal{L}\left(L^2(N^*_\sigma\Lambda)\right). \tag{9.3.12}$$

Observe that saying that $\mathfrak{m}$ is a measure on $\mathbb{R} \times E\Lambda$ is equivalent to defining M as a measure on $\mathbb{R} \times T^*\Lambda$ and taking values in $\mathcal{H}\Lambda$ rigidly, *i.e.*, in such a manner that, for $(t, \sigma, v_\sigma) \in \mathbb{R} \times T^*\Lambda$, one have $\mathfrak{M}(t, \sigma, v_\sigma) \in \mathcal{H}_\sigma\Lambda$ (see Remark 2.3.3).

9.4 The two-microlocal Wigner measures

9.4.1 The measures' geometric character

In this section we will describe the transformations that the semiclassical measures and the pseudodifferential operators undergo by passing from Λ to Λ_0 through the diffeomorphism κ between Ω and Ω_0 and the corresponding change $\tilde{\kappa}$ between $T^*\Omega$ and $T^*\Omega_0$:

$$\tilde{\kappa}(x,\xi) = \left({}^t\nabla\kappa(\xi)^{-1}x, \kappa(\xi)\right), \tag{9.4.1}$$

which will further be justified in the proof of Proposition 9.4.1 ahead; we also study the change between different charts of Ω_0, which is rather similar.

Below we will use the unitary ε-Fourier transform defined as:

$$\mathcal{F}_\varepsilon\Psi(\xi) = \frac{1}{(2\pi\varepsilon)^{d/2}}\int \mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi}\Psi(x)\,dx \quad \forall\,\Psi\in L^2(\mathbb{R}^d), \tag{9.4.2}$$

and we will extend κ diffeomorphically to the whole $\mathbb{R}^d$.

Proposition 9.4.1. *Let be κ a diffeomorphism of $\mathbb{R}^d$ in the sense of manifolds, and $\tilde{\kappa}$ as defined in* (9.4.1). *Then, for $a\in C_0^\infty\left(\mathbb{R}^{2d}\right)$, one has*

$$\langle \mathrm{op}_\varepsilon(a)u_t^\varepsilon, u_t^\varepsilon\rangle = \left\langle \mathrm{op}_\varepsilon\left(a\circ\tilde{\kappa}^{-1}\right)T_{\tilde{\kappa}}^\varepsilon u_t^\varepsilon, T_{\tilde{\kappa}}^\varepsilon u_t^\varepsilon\right\rangle + \varepsilon\, N_{d+1}(a),$$

where $N_d(a)$ is a seminorm for a like those in (2.1.2) *and* (2.1.3)*, and $T_{\tilde{\kappa}}^\varepsilon = \mathcal{F}_\varepsilon^*\,T_\kappa\,\mathcal{F}_\varepsilon$ is an unitary operator on $L^2(\mathbb{R}^d)$, with T_κ given as in formula 9.4.4.*

Proof. Let us recall that the phase space $\mathbb{R}^{2d}$ has the structure of the cotangent bundle $T^*\mathbb{R}^d$ at the same time as a symplectic structure induced by the canonical form $dx\wedge d\xi$. Posing the symplectic change of variables $\omega(x,\xi) = (\xi,-x)$, for any symbol $a\in C_0^\infty(\mathbb{R}^{2d})$ one has, after a short calculation:

$$\mathrm{op}_\varepsilon(a\circ\omega) = \mathcal{F}_\varepsilon^*\,\mathrm{op}_\varepsilon(a)\,\mathcal{F}_\varepsilon.$$

According to Proposition 4.1.2 in Part II of this thesis, for a cotangent coordinate change $\tilde{\phi}(x,\xi) = \left(\phi(x), {}^t\nabla\phi(x)^{-1}\xi\right)$, with ϕ a global diffeomorphism, one has:

$$\left\|\mathrm{op}_\varepsilon(a) - T_\phi^*\,\mathrm{op}_\varepsilon(a\circ\tilde{\phi}^{-1})\,T_\phi\right\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \leqslant \varepsilon\, C \sup_{\substack{\alpha,\beta\in\mathbb{N}_0^d\\ |\alpha|+|\beta|\leqslant 1}} N_d\left(\partial_x^\alpha\partial_\xi^\beta a\right), \tag{9.4.3}$$

where the constant C is independent of a and where T_ϕ is the unitary operator defined as

$$T_\phi\Psi = \left(J_\phi\circ\phi^{-1}\right)^{-\frac{1}{2}}\Psi\circ\phi^{-1} \quad \text{for } \Psi\in L^2(\mathbb{R}^d), \tag{9.4.4}$$

J_ϕ is the Jacobian of ϕ. For subsequent coordinate changes $\phi_1\circ\phi_2\circ...\circ\phi_j$, with $j\in\mathbb{N}$, one has $T_{\phi_1\phi_2...\phi_j} = T_{\phi_1}T_{\phi_2}...T_{\phi_j}$ and $T_{\phi^{-1}} = T_\phi^{-1}$; writing $T_\omega = \mathcal{F}_\varepsilon$, then ω can be included in this group.

Furthermore, we can canonically extend κ to the phase space over $\mathcal{A}$ by doing:

$$\tilde{\kappa} \,:\, (x,\xi) \underset{\omega}{\longmapsto} (\xi,-x) \underset{\kappa}{\longmapsto} \left(\kappa(\xi), -{}^t\nabla\kappa(\xi)^{-1}x\right) \underset{\omega^{-1}}{\longmapsto} \left({}^t\nabla\kappa(\xi)^{-1}x, \kappa(\xi)\right).$$

It follows that

$$T_{\tilde{\kappa}}^\varepsilon = \mathcal{F}_\varepsilon^*\,T_\kappa\mathcal{F}_\varepsilon, \tag{9.4.5}$$

which is also an unitary operator. □

From the proof above, in particular from estimate (9.4.3) and identity (9.4.5), we get:

Scholium 9.4.2. *Let be ϑ be a diffeomorphism of $\mathbb{R}^d$ in the sense of manifolds, and $\tilde{\vartheta}$ its extension to the cotangent bundle as in* (9.3.4). *Then, there exists a constant $C > 0$ such that, for any $a \in S(p)$, we have:*

$$\left\| \mathrm{op}_\varepsilon^\sharp(a) - T_{\tilde{\vartheta}}^{\varepsilon *} \,\mathrm{op}_\varepsilon \left(a_\varepsilon^\sharp \circ \tilde{\vartheta}^{-1} \right) T_{\tilde{\vartheta}}^{\varepsilon} \right\|_{\mathcal{L}\left(L^2(\mathbb{R}^d)\right)} \leqslant \varepsilon\, C \sup_{\substack{\alpha,\beta \in \mathbb{N}_0^{d-p} \\ |\alpha|+|\beta| \leqslant 1}} N_d\left(\partial_{x'}^\alpha \partial_{\xi'}^\beta a \right),$$

where $T_{\tilde{\vartheta}}^\varepsilon = \mathcal{F}_\varepsilon^* \, T_\vartheta \, \mathcal{F}_\varepsilon$ with T_ϑ defined as in (9.4.4)*, $a_\varepsilon^\sharp$ is such that $\mathrm{op}_\varepsilon^\sharp(a) = \mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp\right)$, and N_d is the seminorm in* (2.1.2).

This result is kind of a specialization of Proposition 9.4.1 for a "pure" change of coordinates between charts $\kappa_1, \kappa_2 \in \mathcal{A}$ with (the extension to the whole $\mathbb{R}^d$ of) a transition function $\vartheta = \kappa_1 \circ \kappa_2^{-1}$, which is a local diffeomorphism with domain on some $V \subset \mathbb{R}^d$ and extends to the phase space around V as the cotangent variable change $\tilde{\vartheta}$ in (9.3.4).

Let us now use this fact to prove that the two-microlocal measures are geometric objects defined on some bundles of Λ:

Corollary 9.4.3. *Let be $\mathbb{A}'$ is an atlas for Λ and $(u^\varepsilon)_{\varepsilon>0} \subset L^2(\mathbb{R}^d)$ uniformly bounded. Then, the families $(\nu_\kappa)_{\kappa' \in \mathbb{A}'}$ and $(M_\kappa)_{\kappa' \in \mathbb{A}'}$, obtained from the two-microlocalization of $(T_{\tilde{\kappa}}^\varepsilon u^\varepsilon)_{\varepsilon>0}$ as in Proposition 9.1.2, define a measure ν on $\mathbb{R} \times SE\Lambda$ and a measure M on $\mathbb{R} \times T^*\Lambda$ taking values in the trace class operators of $\mathcal{H}\Lambda$ in such a manner that, for $(t, \sigma, v_\sigma) \in \mathbb{R} \times T^*\Lambda$, $\mathfrak{M}(t, \sigma, v_\sigma) \in \mathcal{H}_\sigma\Lambda$.*

Proof. Let be $\kappa_1, \kappa_2 \in \mathbb{A}$ with $\Lambda \cap V_1 \cap V_2 \neq \emptyset$; as we saw in section 9.3, passing from Λ to Λ_0 in chart κ induces a phase space transformation $\tilde{\kappa}$ in (9.3.4) and, in other bundles of Λ_0, other transformations, in particular κ_E and κ_{SE} respectively for the bundles in (9.3.10) and (9.3.11). Define the transition function $\vartheta = \kappa_1 \circ \kappa_2^{-1}$, extend everything diffeomorphically to the whole $\mathbb{R}^d$, and notice that $T_{\tilde{\vartheta}}^\varepsilon = T_{\tilde{\kappa}_1}^\varepsilon \, T_{\tilde{\kappa}_2}^{\varepsilon\;-1}$.

Moreover, for any $a \in S(p)$ define $a_\varepsilon^\sharp$ so as $\mathrm{op}_\varepsilon^\sharp(a) = \mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp\right)$; from Scholium 9.4.2 we get:

$$\begin{aligned} \left\langle \mathrm{op}_\varepsilon \left(a_\varepsilon^\sharp \circ \tilde{\kappa}_2^{-1} \right) T_{\tilde{\kappa}_2}^\varepsilon u_t^\varepsilon, T_{\tilde{\kappa}_2}^\varepsilon u_t^\varepsilon \right\rangle &= \left\langle \mathrm{op}_\varepsilon \left(a_\varepsilon^\sharp \circ \tilde{\kappa}_2^{-1} \circ \tilde{\vartheta}^{-1} \right) T_{\tilde{\vartheta}}^\varepsilon \, T_{\tilde{\kappa}_2}^\varepsilon u_t^\varepsilon, T_{\tilde{\vartheta}}^\varepsilon \, T_{\tilde{\kappa}_2}^\varepsilon u_t^\varepsilon \right\rangle + \mathcal{O}(\varepsilon) \\ &= \left\langle \mathrm{op}_\varepsilon \left(a_\varepsilon^\sharp \circ \tilde{\kappa}_1^{-1} \right) T_{\tilde{\kappa}_1}^\varepsilon u_t^\varepsilon, T_{\tilde{\kappa}_1}^\varepsilon u_t^\varepsilon \right\rangle + \mathcal{O}(\varepsilon), \end{aligned}$$

which already hints the chart independence of the two-microlocal measures to come, hence their geometric nature. Finally, pick up $\Xi \in \mathcal{C}_0^\infty(\mathbb{R})$ and observe:

- taking first a compactly supported in all variables and denoting $\tilde{a}(z, \zeta', \rho) = a(z, \zeta', 0, \rho)$, we deduce:

$$\mathrm{tr} \int_{\mathbb{R} \times \mathbb{R}^{2(d-p)}} \Xi(t) \left(\tilde{a} \circ \kappa_{E,2}^{-1} \right)^W (z', y, \zeta', \partial_y)\, M_{\kappa_2}(dt, dz', d\zeta') =$$
$$\mathrm{tr} \int_{\mathbb{R} \times \mathbb{R}^{2(d-p)}} \Xi(t) \left(\tilde{a} \circ \kappa_{E,1}^{-1} \right)^W (z', y, \zeta', \partial_y)\; M_{\kappa_1}(dt, dz', d\zeta')$$

  (y is a dummy variable to represent that this operator acts on $L^2(N_\sigma^*\Lambda_0)$), which gives a measure

$$\mathrm{tr} \left\langle \tilde{M}(t, \sigma, v_\sigma)\,,\, \Xi(t)\, \left(\tilde{a} \circ \kappa_E^{-1} \right)^W (\sigma, v_\sigma) \right\rangle_{\mathbb{R} \times T^*\Lambda_0}, \tag{9.4.6}$$

  $\left(\tilde{a} \circ \kappa_E^{-1} \right)^W$ being the Weyl quantization of $(z'', \zeta'') \longrightarrow \tilde{a} \circ \kappa_E^{-1}(v_\sigma, z'', \sigma, \zeta'')$;

- taking now any $a \in S(p)$ homogeneous of order 0 in the last variable and denoting $\tilde{a}_\infty(z,\zeta',\omega) = a_\infty(z,\zeta',0,\omega)$, we get:

$$\int_{\mathbb{R}\times\mathbb{R}^{2d-p}\times\mathcal{S}^{p-1}} \Xi(t)\,\tilde{a}_\infty \circ \kappa_{SE,2}^{-1}(z,\zeta',\omega)\,\nu_{\kappa_2}(dt,dz,d\zeta',d\omega) = \int_{\mathbb{R}\times\mathbb{R}^{2d-p}\times\mathcal{S}^{p-1}} \Xi(t)\,\tilde{a}_\infty \circ \kappa_{SE,1}^{-1}\,(z,\zeta',\omega)\;\nu_{\kappa_1}(dt,dz,d\zeta',d\omega),$$

giving

$$\left\langle\, \tilde{\nu}\,(t,v_\sigma,w_\sigma,\sigma,\omega_\sigma)\;,\;\Xi(t)\,\tilde{a}_\infty \circ \kappa_{SE}^{-1}\,(v_\sigma,w_\sigma,\sigma,\omega_\sigma)\,\right\rangle_{\mathbb{R}\times SE\Lambda_0}. \tag{9.4.7}$$

Pulling back $\tilde{M}$ and $\tilde{\nu}$ from Λ_0 to Λ through diffemorphism (9.3.2), we obtain measures M and ν as stated, where (9.4.6) and (9.4.7) become

$$\operatorname{tr}\left\langle\, M(t,\sigma,v_\sigma)\,,\,\Xi(t)\,\tilde{a}^W(\sigma,v_\sigma)\,\right\rangle_{\mathbb{R}\times T^*\Lambda} \tag{9.4.8}$$

and

$$\left\langle\, \nu\,(t,v_\sigma,w_\sigma,\sigma,\omega_\sigma)\;,\;\Xi(t)\,\tilde{a}_\infty\,(v_\sigma,w_\sigma,\sigma,\omega_\sigma)\,\right\rangle_{\mathbb{R}\times SE\Lambda}. \tag{9.4.9}$$

Nonetheless, we still need to show that M and ν are effectively the two-microlocal measures linked to the concentration of $(u^\varepsilon)_{\varepsilon>0}$, *i.e.*, that the Wigner measure μ of u^ε admits a decomposition of the kind (2.3.3) in Lemma 2.3.7 in terms of these M and ν.

This should be obvious by now, not only because $\tilde{M}$ and $\tilde{\nu}$ decompose $\tilde{\mu}$, the semi-classical measure of $(T^\varepsilon_{\tilde{\kappa}}u^\varepsilon)_{\varepsilon>0}$ (which is, by Proposition 9.4.1, a push-forward of μ), but also because, speaking more directly, Scholium 9.4.2 remains valid for arbitrary diffeomorphisms when restricted to the special symbols of $S(p)$ that are constant in the third variable, which actually turn out to be $C_0^\infty(\mathbb{R}^{2d})$. For them, we have the identity $\mathrm{op}^\sharp_\varepsilon(a) = \mathrm{op}_\varepsilon(a)$ and, therefore (recalling the definition of $\mathrm{op}_\varepsilon(a^\sharp_\varepsilon) = \mathrm{op}^\sharp_\varepsilon(a)$):

$$\langle \mathrm{op}_\varepsilon(a)u^\varepsilon_t, u^\varepsilon_t\rangle = \left\langle \mathrm{op}_\varepsilon\left(a^\sharp_\varepsilon \circ \tilde{\kappa}^{-1}\right) T^\varepsilon_{\tilde{\kappa}}u^\varepsilon_t, T^\varepsilon_{\tilde{\kappa}}u^\varepsilon_t\right\rangle + \mathcal{O}(\varepsilon),$$

which is nothing else than the result we wanted. □

Remark 9.4.4. This last proof also works for Corollary 4.1.3 in Chapter 4, Section 4.1, since the geodesic coordinates presented in (9.3.1) also apply to that case (and, in fact, to many other submanifolds). This particular construction does not imply any loss of generality, since what is needed in order to understand the geometric behaviour of mathematical objects over the bundles of Λ is actually generality in the choice of the atlas $\mathbb{A}'$, which we indeed have got, and not in the choice of an $\mathbb{A}$ for Ω, which was only an accessory to ease the description of Λ within Ω.

Before we can proceed to the actual analysis of $\tilde{u}^\varepsilon = T^\varepsilon_{\tilde{\kappa}}u^\varepsilon$, one more result is to be stated:

Proposition 9.4.5. *Suppose that u^ε satisfies equation* (9.1.1) *and $T^\varepsilon_{\tilde{\kappa}}$ is the operator given in Proposition 9.4.1. Then, setting $|t| \leqslant T$ and $\tilde{u}^\varepsilon_t = T^\varepsilon_{\tilde{\kappa}}u^\varepsilon_t$, $\tilde{u}^\varepsilon$ obeys to the equation*

$$i\varepsilon^2\partial_t\tilde{u}^\varepsilon(t,z) = \tilde{\lambda}(\varepsilon\partial_z)\tilde{u}^\varepsilon(t,z) + \varepsilon^2\mathrm{op}_\varepsilon\,(b)\,\tilde{u}^\varepsilon(t,z) + \mathcal{O}_{L^2(\mathbb{R}^d)}(\varepsilon^3), \tag{9.4.10}$$

where $\tilde{\lambda}(\zeta) = \lambda \circ \kappa^{-1}(\zeta)$ and $b(z,\zeta) = V\left({}^t\nabla\kappa \circ \kappa^{-1}(\zeta)\,z\right)$.

Proof. Remark that $\mathcal{F}_\varepsilon \tilde{u}^\varepsilon = T_\kappa \mathcal{F}_\varepsilon u^\varepsilon$; denoting $\hat{u}^\varepsilon = \mathcal{F}_\varepsilon \tilde{u}^\varepsilon$, passing (8.3.1) to the Fourier space with $\mathcal{F}_\varepsilon$, multiplying both sides by T_κ and staying within compact times $|t| \leqslant T$:

$$i\varepsilon^2 \dot{\hat{u}}^\varepsilon(t,\zeta) = \lambda \circ \kappa^{-1}(\zeta)\hat{u}^\varepsilon(t,\zeta) + \varepsilon^2\, T_\kappa\, V\left(-\varepsilon\partial_\xi\right)\, T_\kappa^*\, \hat{u}^\varepsilon(t,\zeta) + \mathcal{O}_{L^2(\mathbb{R}^d)}(\varepsilon^3),$$

where $V\left(-\varepsilon\partial_\xi\right)$ is the Weyl quantization of the symbol $(\xi,x) \longmapsto V(-x)$. By Proposition 9.4.1, it follows that

$$T_\kappa\, V\left(-\varepsilon\partial_\xi\right)\, T_\kappa^* = \mathrm{op}_\varepsilon\left(b(\zeta,-z)\right) + \mathcal{O}_{L^2(\mathbb{R}^d)}(\varepsilon),$$

with $b(\zeta,z) = V \circ \tilde{\kappa}^{-1}(z,\zeta)$. The conclusion comes from passing back to the position space with $\mathcal{F}_\varepsilon^*$. □

This section has enabled us to study the two-microlocal concentration of a family $(\tilde{u}^\varepsilon)_{\varepsilon>0}$ satisfying (9.4.10) over the vector space $\{\zeta'' = 0\}$, and then to transpose the results to $(u^\varepsilon)_{\varepsilon>0}$ over Λ.

9.4.2 Properties of the measure at infinity ν

Denote by $B(\sigma)$ the bilinear form on $N_\sigma\Lambda$ induced by the projection of $\nabla^2\lambda(\sigma)$; in a chart κ where the coordinates of η_σ are ρ and those of σ are ζ', one has $\kappa_N\left(B(\sigma)\eta_\sigma\right) = \nabla^2_{\zeta''}\tilde{\lambda}(\zeta',0)\rho$. Additionally, $B(\sigma)\eta_\sigma$ is a linear form on $N_\sigma\Lambda$ and consequently an element of $N_\sigma^*\Lambda$, so the flow in next lemma is well-defined.

Lemma 9.4.6. *For $\sigma \in \Lambda$, $v_\sigma \in T_\sigma^*\Lambda$, $w_\sigma \in N_\sigma^*\Lambda$ and $\eta_\sigma \in N_\sigma\Lambda$, define the following flow in $SE\Lambda$:*

$$\Phi_s\ :\ \left(v_\sigma, w_\sigma, \sigma, \frac{\eta_\sigma}{\|\eta_\sigma\|}\right) \longmapsto \left(v_\sigma, w_\sigma + sB(\sigma)\eta_\sigma, \sigma, \frac{\eta_\sigma}{\|\eta_\sigma\|}\right).$$

Measure ν is invariant by this flow Φ_s.

Proposition 9.4.7. *If the Hessian of λ is of maximal rank on the critical set Λ, then $\nu = 0$.*

The proof of Proposition 9.4.7 follows the lines of Proposition 9.1.1, since the maximal rank condition implies that the map $N_\sigma\Lambda \ni \eta \longmapsto B(\sigma)\eta \in N_\sigma^*\Lambda$ is injective, then Φ is dispersive. Let us now prove the lemma.

Proof. Set the flow $\tilde{\Phi}$ on the bundle of fibres $V_\sigma\Lambda_0 = E_\sigma\Lambda_0 \oplus N_\sigma\Lambda_0$, defined in a chart $\kappa \in \mathbb{A}$ by:

$$\kappa_V \circ \tilde{\Phi}_s \circ \kappa_V^{-1}\ :\ \left(z', z'', \zeta', \zeta'', \rho\right) \longmapsto \left(z', z'' + s\,\nabla^2_{\zeta''}\lambda(\zeta',0)\,\zeta'', \zeta', \zeta'', \rho\right).$$

Consider an observable $a \in S(p)$ and let be

$$a_{R,\delta} \circ \kappa_V^{-1}(z,\zeta,\rho) = a \circ \kappa_V^{-1}(z,\zeta,\rho)\left(1 - \chi\left(\frac{\rho}{R}\right)\right)\chi\left(\frac{\zeta''}{\delta}\right),$$

with χ a cut-off as usual.

It follows that

$$\frac{d}{ds}\left(\left(a_{R,\delta} \circ \tilde{\Phi}_s\right) \circ \kappa_V^{-1}\right)\Big|_{s=0} = \nabla_z\left(a_{R,\delta} \circ \kappa_V^{-1}\right) \cdot \nabla^2_\zeta\tilde{\lambda}(\zeta',0)\begin{pmatrix} 0 \\ \zeta'' \end{pmatrix}.$$

Using a Taylor expansion and remembering that $\nabla\tilde{\lambda}(\zeta',0)=0$, we can write

$$\nabla\tilde{\lambda}(\zeta)=\nabla_\zeta^2\tilde{\lambda}(\zeta',0)\begin{pmatrix}0\\ \zeta''\end{pmatrix}+\Gamma(\zeta)\left(\zeta''\right)^{(2)},$$

where Γ is a smooth tensor of order 3 such that

$$\mathrm{op}_\varepsilon^\sharp\left(\nabla_z\left(a_{R,\delta}\circ\kappa_V^{-1}\right)\cdot\Gamma(\zeta)\left(\zeta''\right)^{(2)}\right)=\mathcal{O}\left(\varepsilon^2\right).$$

Thus, considering (9.4.10), we get

$$\begin{aligned}
&\mathrm{op}_\varepsilon^\sharp\left(\frac{d}{ds}\left((a_{R,\delta}\circ\tilde{\Phi}_s)\circ\kappa_V^{-1}\right)\Big|_{s=0}\right)\\
=\;&\mathrm{op}_\varepsilon^\sharp\left(\nabla_z\left(a_{R,\delta}\circ\kappa_V^{-1}\right)\cdot\nabla_\zeta\tilde{\lambda}(\zeta)\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right)\\
=\;&\frac{i}{\varepsilon}\left[\tilde{\lambda}(\varepsilon\partial_z)\,,\,\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\circ\kappa_V^{-1}\right)\right]+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right)\\
=\;&\frac{i}{\varepsilon}\left[\tilde{\lambda}(\varepsilon\partial_z)+\varepsilon^2\mathrm{op}_\varepsilon(b)\,,\,\mathrm{op}_\varepsilon^\sharp\left(a_{R,\delta}\circ\kappa_V^{-1}\right)\right]+\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right)
\end{aligned}$$

As a result, for any $\Xi\in C_0^\infty(\mathbb{R})$,

$$\begin{aligned}
&\int_{\mathbb{R}}\Xi(t)\left\langle\mathrm{op}_\varepsilon^\sharp\left(\frac{d}{ds}\left((a_{R,\delta}\circ\tilde{\Phi}_s)\circ\kappa_V^{-1}\right)\Big|_{s=0}\right)\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle dt\\
=\;&\varepsilon\int_{\mathbb{R}}\Xi(t)\frac{d}{dt}\left\langle\mathrm{op}_\varepsilon^\sharp\left((a_{R,\delta}\circ\tilde{\Phi}_s)\circ\kappa_V^{-1}\right)\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle dt+\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right)\\
=\;&-\varepsilon\int_{\mathbb{R}}\Xi'(t)\left\langle\mathrm{op}_\varepsilon^\sharp\left((a_{R,\delta}\circ\tilde{\Phi}_s)\circ\kappa_V^{-1}\right)\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle dt+\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right)\\
=\;&\mathcal{O}\left(\varepsilon\right)+\mathcal{O}\left(\frac{\varepsilon}{\delta}\right)+\mathcal{O}\left(\frac{1}{R}\right)+\mathcal{O}\left(\delta\right).
\end{aligned}$$

Finally, taking the limits $\varepsilon\to 0$, then $R\to\infty$ and last $\delta\to 0$, we conclude that

$$\int_{\mathbb{R}\times\mathbb{R}^{2d-p}\times\mathcal{S}^{p-1}}\Xi(t)\left(\frac{d}{ds}\left(\tilde{a}_\infty\circ\Phi_s\right)\Big|_{s=0}\right)\circ\kappa_{SE}^{-1}(z,\zeta',\omega)\,\nu_\kappa(dt,dz,d\zeta',d\omega)=0$$

for all charts $\kappa\in\mathbb{A}$, with $\tilde{a}_\infty(z,\zeta',\omega)=a_\infty(z,\zeta',0,\omega)$. Finally, back to ν on $SE\Lambda$:

$$\int_{\mathbb{R}\times SE\Lambda}\Xi(t)\,\frac{d}{ds}\left(a_\infty\circ\Phi_s\right)\Big|_{s=0}d\nu=0.$$

This proves the lemma. □

9.4.3 Properties of the operator-valued measure M

Let us now consider the operator-valued measure M.

Proposition 9.4.8. *One has the decomposition $M(t,\sigma,v_\sigma)=\mathfrak{M}(t,\sigma,v_\sigma)\gamma(\sigma,v_\sigma)dt$ as in Remark 9.1.4, with γ not depending on t. Furthermore, the function $\mathbb{R}\ni t\longmapsto\mathfrak{M}(t,\cdot)\in L^\infty\left(T^*\Lambda,\mathcal{H}\Lambda\right)$ is continuous and obeys to:*

$$\begin{cases}i\partial_t\mathfrak{M}(t,\sigma,v_\sigma)=\left[-\frac{1}{2}B(\sigma)\partial_{w_\sigma}\cdot\partial_{w_\sigma}+V\left(v_\sigma+w_\sigma\right)\,,\,\mathfrak{M}(t,\sigma,v_\sigma)\right]\\ \mathfrak{M}(0,\sigma,v_\sigma)=\mathfrak{M}_0(\sigma,v_\sigma),\end{cases}$$

where $\sigma \in \Lambda$, $v_\sigma \in T^*_\sigma\Lambda$, $w_\sigma \in N^*_\sigma\Lambda$, and $\mathfrak{M}_0$ is the operator-valued part of the microlocal measure associated to the concentration of $(u_0^\varepsilon)_{\varepsilon>0}$ chosen in order to satisfy

$$\mathrm{tr}_{L^2(N^*_\sigma\Lambda)}\mathfrak{M}_0(\sigma, v_\sigma) = 1.$$

Proof. Let us work on a chart κ of Λ_0. Consider a symbol $a \in C_0^\infty\left(\mathbb{R}^{2d+p}\right)$, write $a_\varepsilon^\sharp$ as usual and calculate from (9.4.10):

$$\frac{d}{dt}\left\langle \mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp \circ \kappa^{-1}\right)\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle = \left\langle \frac{i}{\varepsilon^2}\left[\tilde{\lambda}(\varepsilon\partial_z) + \varepsilon^2\mathrm{op}_\varepsilon(b)\,,\,\mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp \circ \kappa^{-1}\right)\right]\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle + \mathcal{O}(\varepsilon).$$

Using a Taylor expansion, we have:

$$\tilde{\lambda}(\zeta', \zeta'') = \tilde{\lambda}(\zeta', 0) + \nabla_{\zeta''}\tilde{\lambda}(\zeta', 0)\zeta'' + \frac{1}{2}\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)\zeta'' \cdot \zeta'' + \mathcal{O}\left(\zeta''^{(3)}\right),$$

and recalling that, since $\nabla\lambda$ is null over Λ, $\nabla\tilde{\lambda}(\zeta', 0) = 0$ for any ζ' and, as a consequnce, $\tilde{\lambda}(\zeta', 0) = \tilde{\lambda}(\zeta'_0, 0)$ for $\zeta'_0 = \kappa(\sigma_0)$ with some $\sigma_0 \in \Lambda$, which implies that $\mathrm{op}_\varepsilon(\tilde{\lambda}(\zeta', 0))$ is just $\lambda(\sigma_0)\mathbb{1}$; it follows that:

$$\frac{d}{dt}\left\langle \mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp \circ \kappa^{-1}\right)\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle =$$
$$\left\langle i\left[\mathrm{op}_\varepsilon\left(\frac{1}{2}\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)\frac{\zeta''}{\varepsilon} \cdot \frac{\zeta''}{\varepsilon} + b(z, \zeta)\right)\,,\,\mathrm{op}_\varepsilon\left(a_\varepsilon^\sharp \circ \kappa^{-1}\right)\right]\tilde{u}_t^\varepsilon\,,\,\tilde{u}_t^\varepsilon\right\rangle + \mathcal{O}(\varepsilon),$$

which implies the time continuity of the measure M in the same way as it happened in Lemma 9.2.1. Finally, choosing $\Xi \in C_0^\infty(\mathbb{R})$, writing $\tilde{a}(z, \zeta', \rho) = a(z, \zeta', 0, \rho)$ and taking the limit $\varepsilon \longrightarrow 0$:

$$\mathrm{tr}\int_{\mathbb{R}\times\mathbb{R}^{2(d-p)}} \Xi(t)\,\left(\tilde{a} \circ \kappa_E^{-1}\right)^W(z', y, \zeta', \partial_y)\,\partial_t M_\kappa(dt, dz', d\zeta') =$$
$$\mathrm{tr}\int_{\mathbb{R}\times\mathbb{R}^{2(d-p)}} \Xi(t) i\left[-\frac{1}{2}\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)\partial_y \cdot \partial_y + b(z', y, \zeta', 0)\,,\right.$$
$$\left.\left(\tilde{a} \circ \kappa_E^{-1}\right)^W(z', y, \zeta', \partial_y)\right] M_\kappa(dt, dz', d\zeta'),$$

implying the equation

$$i\partial_t M_\kappa(t, z', \zeta') = \left[-\frac{1}{2}\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)\partial_y \cdot \partial_y + b(z', y, \zeta', 0)\,,\,M_\kappa(t, z', \zeta')\right],$$

which admits the solution $M(t, z', \zeta') = \mathfrak{M}(t, z', \zeta')\gamma(z', \zeta')dt$, where γ is time-independent and $\mathfrak{M}$ is a solution to

$$i\partial_t\mathfrak{M}_\kappa(t, z', \zeta') = \left[-\frac{1}{2}\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)\partial_y \cdot \partial_y + b(z', y, \zeta', 0)\,,\,\mathfrak{M}_\kappa(t, z', \zeta')\right]$$

inside the local chart.

Now, we recognize z' as the coordinate of $v_\sigma \in T^*_\sigma\Lambda_0$, ζ' as that of $\sigma \in \Lambda_0$, and y as that of the dummy $w_\sigma \in N^*_\sigma\Lambda$; recalling (9.3.7) and (9.3.8), we have

$$b(z, \zeta) = V\left({}^t\nabla\kappa \circ \kappa^{-1}(\zeta)\,z\right) = V(v_\sigma + w_\sigma),$$

and the proposition follows from recognizing $\nabla^2_{\zeta''}\tilde{\lambda}(\zeta', 0)$ as the bilinear form $B(\sigma)$ on $N^*_\sigma\Lambda$ in the chart κ.

Last, remember that the decomposition $M = \mathfrak{M}\gamma$ is not unique, as we explained in Remark 9.1.4. The condition $\mathrm{tr}_{L^2(N^*_\sigma\Lambda)}\mathfrak{M}_0(\sigma, v_\sigma) = 1$ in the proposition's statement allows us to fix the constant C in that remark and to be unambiguous with respect to $\mathfrak{M}_0$ and its evolution over the time. □

Remark 9.4.9. Since $\|u_t^\varepsilon\|_{L^2(\mathbb{R}^d)} = 1$ uniformly in ε, it is easy to show that

$$\int_{T^*\Lambda} \mathrm{tr}_{N_\sigma^*\Lambda}\, \mathfrak{M}(t,\sigma,v_\sigma)\, \gamma(d\sigma, dv_\sigma) = 1$$

for every $t \in \mathbb{R}$. Since we chose $\mathrm{tr}_{N_\sigma^*\Lambda}\, \mathfrak{M}_0(\sigma, v_\sigma) = 1$, it follows that $\int_{T^*\Lambda} \gamma(d\sigma, dv_\sigma) = 1$, which is a good normalization for γ, that will describe the problem's mass distribution over the phase space.

9.5 Collating results

At this proint, proving Theorem 8.3.4 is very easy. Proposition 9.4.7 holds under hypothesis **w-H2**, besides, if we are to study the limits of an expression like

$$\int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)\, |u^\varepsilon(t,x)|^2\, dx\, dt,$$

with $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, **H0** permits that we do so with the Wigner measures by projecting them in the position space. Since in this case we are left solely with M, we will have

$$\mathrm{tr} \int_{\mathbb{R}\times T^*\Lambda} \phi^W(t,\sigma,v_\sigma)\, \mathfrak{M}(t,\sigma,v_\sigma)\gamma(d\sigma, dv_\sigma)dt,$$

where $\phi^W(t,\sigma,v_\sigma) \in \mathcal{L}\left(L^2(N_\sigma^*\Lambda)\right)$ is the Weyl quantization of the symbol $(\sigma, v_\sigma) \longmapsto \phi(t, v_\sigma, w_\sigma)$, $w_\sigma \in N_\sigma^*\Lambda$ being a dummy variable, which after a short calculation we find out to be just the multiplication by $\phi\,(t, \varpi)$, with $\varpi = v_\sigma + w_\sigma \in \mathbb{R}^d$ as in Remark 9.3.3.

This is precisely what is said in the theorem. The other properties of $\mathfrak{M}$ are listed in Proposition 9.4.8.

Chapter 10

The equations of effective mass

10.1 Time localized analysis

Here we are going to need semiclassical measures for families $(\Psi^\varepsilon)_{\varepsilon>0}$ (of solutions to a certain evolution equation) which are bounded in $L^\infty\left(\mathbb{R}, L^2(\mathbb{R}^d)\right)$ and, therefore, only locally integrable with respect to the first variable t. It will thus be convenient to introduce a localized-in-time Wigner transform:

$$\widetilde{W}^\varepsilon\Psi^\varepsilon(t,\tau,x,\xi) = \frac{1}{(2\pi\varepsilon)^{d+1}}\int_{\mathbb{R}^{d+1}} e^{\frac{i}{\varepsilon}(\xi\cdot y-\tau\cdot s)}\Psi^\varepsilon\left(t-\frac{s}{2},x-\frac{y}{2}\right)\overline{\Psi^\varepsilon\left(t+\frac{s}{2},x+\frac{y}{2}\right)}\,ds\,dy, \tag{10.1.1}$$

acting on test functions $a \in C_0^\infty(\mathbb{R}^2_{t,\tau}\times\mathbb{R}^{2d}_{x,\xi})$ through the identity

$$\left\langle \widetilde{W}^\varepsilon_\phi\Psi^\varepsilon\,,\,a\right\rangle_{\mathbb{R}^{2(d+1)}} = \langle\, \widetilde{\mathrm{op}}_\varepsilon(a^\varepsilon)\,\phi\Psi^\varepsilon\,,\phi\Psi^\varepsilon\,\rangle_{L^2(\mathbb{R}^{d+1})}\,, \tag{10.1.2}$$

where $\phi\in C_0^\infty(\mathbb{R})$, a^ε stands for $a^\varepsilon(t,\tau,x,\xi)=a(t,\varepsilon\tau,x,\xi)$ and, naturally, we define the time localized pseudodifferential operator of symbol a as:

$$\widetilde{\mathrm{op}}_\varepsilon(a)f^\varepsilon(t,x) = \int_{\mathbb{R}^{2(d+1)}} e^{\frac{i}{\varepsilon}(\xi\cdot(x-y)-\tau\cdot(t-s))}a\left(\frac{t+s}{2},\tau,\frac{x+y}{2},\xi\right)\Psi^\varepsilon(s,y)\,\frac{d\tau\,d\xi\,ds\,dy}{(2\pi\varepsilon)^{d+1}}. \tag{10.1.3}$$

Remark 10.1.1. With these new tools, one can re-write the usual Schrödinger equation as $\widetilde{\mathrm{op}}_\varepsilon(a)\Psi^\varepsilon=0$, with $a(t,\tau,x,\xi)=\tau-\frac{\xi^2}{2}-V(x)$, and the study of its solutions reduces to the analysis of the kernel of $\widetilde{\mathrm{op}}_\varepsilon(a)$. Here, with our special scaling, an equation like $\widetilde{\mathrm{op}}_\varepsilon(a^\varepsilon)\Psi^\varepsilon=0$ with $a(t,\tau,x,\xi)=\tau-\lambda(\xi)-\varepsilon^2V(x)$ gives equation (8.3.1).

The interest of localizing the symbols in τ and t at once will become evident in the proofs of Lemmata 10.2.13 and 10.2.14; it is roughly to assure that one has no interference terms between measures of distinct Bloch modes.

Proposition 10.1.2. *Let the family $(\Psi^\varepsilon)_{\varepsilon>0}$ be bounded in $L^\infty\left(\mathbb{R},L^2(\mathbb{R}^d)\right)$. Then $\left(\widetilde{W}^\varepsilon_\phi\Psi^\varepsilon\right)_{\varepsilon>0}$ in $C_0^\infty(\mathbb{R}^{2(d+1)})$ is uniformly bounded with respect to ε and $\phi\in C_0^\infty(\mathbb{R})$. Moreover, it is possible to extract weakly converging subsequences $\left(\widetilde{W}^{\varepsilon_k}_\phi\Psi^{\varepsilon_k}\right)_{k\in\mathbb{N}}$ such that, for every $\phi\in C_0^\infty(\mathbb{R}^d)$ and every $a\in C_0^\infty(\mathbb{R}^{2(d+1)})$, one has:*

$$\lim_{k\to\infty}\left\langle\widetilde{W}^{\varepsilon_k}_\phi\Psi^{\varepsilon_k}\,,a\right\rangle_{\mathbb{R}^{2(d+1)}} = \int_{\mathbb{R}^{2(d+1)}} a(t,\tau,x,\xi)|\phi(t)|^2\,\widetilde{\mu}(dt,d\tau,dx,d\xi),$$

where the accumulation points $\widetilde{\mu}$ are always positive measures on $\mathbb{R}^{2(d+1)}$. If in addition $(|f^{\varepsilon_k}|^2)_{k\in\mathbb{N}}$ converges in $\mathcal{D}'(\mathbb{R}^{2(d+1)})$ to some measure $\widetilde{\gamma}$, then:

$$\int_{\mathbb{R}^{d+1}} \widetilde{\mu}(\cdot\,, d\tau, \cdot\,, d\xi) \leqslant \widetilde{\gamma},$$

equality taking place if and only if for every $\phi \in C_0^\infty(\mathbb{R})$ the sequence $(\phi\Psi^{\varepsilon_k})_{k\in\mathbb{N}}$ satisfies:

$$\lim_{k\to\infty} \int_{|\varepsilon_k^2\tau|+\|\varepsilon_k\xi\|>R} \left|\widehat{\phi\Psi^{\varepsilon_k}}(\tau,\xi)\right|^2 d\tau d\xi \underset{R\to\infty}{\longrightarrow} 0. \tag{10.1.4}$$

This result's proof can be obtained by following the lines of the proofs of analogous theorems in [55, 56, 58]. Let us now link $\widetilde{\mu}$ with the standard semiclassical measures μ that we have been working with throughout this thesis:

Proposition 10.1.3. *Let $(u^\varepsilon)_{\varepsilon>0}$ be a family of solutions to* (9.1.1) *issued from a sequence of initial data bounded in $L^2(\mathbb{R}^d)$. Suppose $\widetilde{\mu}$ obtained from Proposition 10.1.2 along some subsequence $(\varepsilon_k)_{k\in\mathbb{N}}$. First, one has*

$$\widetilde{\mu}(t,\tau,x,\xi) = \delta\left(\tau - \lambda(\xi)\right) \otimes \widetilde{\nu}(t,x,\xi)$$

for some positive measure $\widetilde{\nu}$ on $\mathbb{R}^{2d+1}$; second, supposing further that μ is the standard semiclassical measure for u^ε through this same sequence ε_k, then, for every $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$:

$$\int_{\mathbb{R}^{2(d+1)}} a(t,\tau,x,\xi)\widetilde{\mu}(dt,d\tau,dx,d\xi) = \int_{\mathbb{R}\times\mathbb{R}^{2d}} a(t,\lambda(\xi),x,\xi)\mu(dt,dx,d\xi).$$

The reader can consult [55] or [78] for a proof of this fact.

10.2 Semiclassical measures for the Bloch decomposition

In this section we will prove Theorem 8.4.2. This will combine three ingredients:

1. We first analyse the high-frequency behaviour of the spectral projectors associated to the Bloch decomposition and of the operator of restriction to the diagonal[1]. Recall that, given any Bloch wave φ_n, we defined in (8.4.1) the operator

$$P^\varepsilon_{\varphi_n}\Psi(x,y) = \varphi_n\left(\varepsilon\partial_x, y\right) \int_{\mathbb{T}^d} \varphi_n\left(\varepsilon\partial_x, z\right)^* \Psi(x,z)\, dz$$

and, according to (8.4.2), for every Bloch eigenvalue λ_j we associated a Bloch spectral projector given by:

$$\Pi^\varepsilon_{\lambda_j} = \sum_{P(\xi)\varphi_n(\xi,\cdot)=\lambda_j(\xi)\varphi_n(\xi,\cdot)} P^\varepsilon_{\varphi_n}.$$

This step will be the object of Section 10.2.1, where, recalling that $\tilde{\Psi}(x,y) = \Psi(x)$ for any $y \in \mathbb{T}^d$, we will prove Proposition 10.2.7 saying that the restriction to the diagonal of the terms $\Pi^\varepsilon_{\lambda_j}\tilde{\Psi}^\varepsilon$ is bounded and ε-oscillating whenever Ψ^ε satisfy these same conditions.

[1] This restriction to the diagonal will take us back from the torus variable y to the fast oscillating $\frac{x}{\varepsilon}$.

2. Secondly, we present the necessary *a priori* estimates that allow us to use a converging Bloch decomposition, in Proposition 10.2.11, and write every solution ψ^ε as:

$$\psi^\varepsilon = \sum_{j\in\mathbb{N}} \psi^\varepsilon_j,$$

where $\psi^\varepsilon_j = \Pi^\varepsilon_{\lambda_j} U^\varepsilon|_{y=\frac{x}{\varepsilon}}$ will be shown in Lemma 10.2.12 to obey to equation (10.2.19), U^ε being a solution to (8.2.2) with initial datum $\tilde{\psi}^\varepsilon_0(x,y) = \psi^\varepsilon_0(x)$. These are the subjects of Section 10.2.2.

3. Finally, the last step consists in computing the semiclassical measures of ψ^ε as the sum of the Wigner measures of the solutions to the dispersive equation (9.1.1) (which were the object of our analysis in the previous chapter) with initial data

$$\psi^\varepsilon_{0,j}(x) = \Pi^\varepsilon_{\lambda_j} \tilde{\psi}^\varepsilon_0\left(x, \frac{x}{\varepsilon}\right).$$

This will be done in Section 10.2.3, where we will prove Proposition 10.2.17, the key result in Part III of this thesis.

10.2.1 Bloch projectors' high-frequency behaviour

Here we will gather some results describing how the ε-oscillation property behaves under the action of the operators $P^\varepsilon_{\varphi_n}$ and the restriction to the diagonal $y = \frac{x}{\varepsilon}$ that are used to recover our solutions ψ^ε on $\mathbb{R}^d$ from the series of Bloch modes on $\mathbb{R}^d \times \mathbb{T}^d$.

It is going to be useful to introduce a notion which is slightly stronger than ε-oscillation. So, let us say that a family $(\Psi^\varepsilon)_{\varepsilon>0}$ in $L^2(\mathbb{R}^d)$ is *strongly ε-oscillating of order $r > 0$* if there exists a constant $C > 0$ independent of ε such that:

$$\forall \varepsilon > 0, \quad \left\| \langle \varepsilon \partial_x \rangle^r \Psi^\varepsilon \right\|_{L^2(\mathbb{R}^d)} \leqslant C, \tag{10.2.1}$$

where $\langle \xi \rangle = \left(1 + |\xi|^2\right)^{\frac{1}{2}}$ as usual.

Remark 10.2.1. If $(\Psi^\varepsilon)_{\varepsilon>0}$ is strongly ε-oscillating of order $r > 0$, then it is easy to see by absurd that, for any $0 \leqslant s < r$, we must have

$$\limsup_{\varepsilon\to 0} \int_{\|\xi\|\geqslant \frac{R}{\varepsilon}} \left| \langle \varepsilon\xi \rangle^s \hat{\Psi}^\varepsilon(\xi) \right|^2 d\xi \underset{R\to\infty}{\longrightarrow} 0.$$

From this limit it is clear that strong ε-oscillation relates to the simple ε-oscillation by, so as to say, changing the $L^2(\mathbb{R}^d)$ norm by that in $H^s_\varepsilon(\mathbb{R}^d)$ with which we estimate the remainder of mass for high frequencies of order larger than $\frac{1}{\varepsilon}$. In particular, if Ψ^ε is strongly ε-oscillating of any strictly positive order, then it is ε-oscillating in the standard sense. For the sake of completeness, let us call it *strong ε-oscillation of order* 0.

Furthermore, write $\|\Psi^\varepsilon\|_{H^r_\varepsilon(\mathbb{R}^d)} = \|\langle \varepsilon\partial_x\rangle^r \Psi^\varepsilon\|_{L^2(\mathbb{R}^d)}$; for a function Q defined on the Cartesian product $\mathbb{R}^d \times \mathbb{T}^d$, we will denote:

$$\|Q\|_{H^r_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} = \|\langle \varepsilon\partial_x\rangle^r Q\|_{L^2\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)}.$$

Remark 10.2.2. Note that for every $s > 0$, the norm $H^s_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$ above defined is thinner than the norm

$$\|P(\varepsilon\partial_x)^s Q\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}$$

uniformly with respect to ε and s, since P is a polynomial of order 2 in ξ and in ∂_y (recall the explicit form of P in (8.2.3)). Analogously, this norm is also thinner than the one in $H^s_\varepsilon\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$.

These notations established, we begin the analysis by proving some boundedness properties for the spectral projectors.

Lemma 10.2.3. *For all $r \geqslant 0$ and $s \geqslant 0$, the operator*

$$P^\varepsilon_{\varphi_n} : H^r_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right) \longrightarrow H^r_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$$

is uniformly bounded with respect to $\varepsilon > 0$.

Proof. Recall that if φ is a Bloch wave, then it satisfies the periodicity condition

$$\varphi(\xi + 2\pi k, y) = e^{-2\pi i k\cdot y}\varphi(\xi, y) \quad \text{for } k \in \mathbb{Z}^d. \tag{10.2.2}$$

Writing

$$c(\xi) = \int_{\mathbb{T}^d} \varphi(\xi, y)dy \tag{10.2.3}$$

and integrating (10.2.2) with respect to y on $\mathbb{T}^d$, one gets the Fourier coefficients of $\varphi(\xi, \cdot\,)$, hence:

$$\varphi(\xi, y) = \sum_{k\in\mathbb{Z}^d} c(\xi + 2\pi k)e^{2\pi i k\cdot y}. \tag{10.2.4}$$

Since $\varphi(\xi, \cdot\,)$ is a smooth function on $\mathbb{T}^d$, its Fourier coefficients must decay faster than any polynomial in k, as we can see from a simple estimation for the norm $L^2(\mathbb{T}^d)$ of $\varphi(\xi, \cdot\,)$ that gives

$$|c(\xi + 2\pi k)| \leqslant \sup_{y\in\mathbb{T}^d} \frac{|\partial_y^\alpha \varphi(\xi, y)|}{|(2\pi k)^\alpha|}, \quad \forall\alpha \in \mathbb{N}_0^d,\ \forall k \in \mathbb{Z}^d_*; \tag{10.2.5}$$

more generally, differentiating identity (10.2.2) gives

$$(-i\partial_y)^\alpha \varphi(\xi - 2\pi j, y) = e^{2\pi i j\cdot y}(2\pi j - i\partial_y)^\alpha \varphi(\xi, y), \quad \forall\alpha \in \mathbb{N}_0^d,\ \forall j \in \mathbb{Z}^d,$$

which, doing the same $L^2(\mathbb{T}^d)$ norm estimation that we did to obtain (10.2.5) for the function $\varphi(\xi - 2\pi j, \cdot\,)$ with its coefficients $c(\xi + 2\pi(k - j))$, results in the estimate:

$$|c(\xi + 2\pi(k - j))| \leqslant \sup_{y\in\mathbb{T}^d} \frac{|(2\pi j - i\partial_y)^\alpha \varphi(\xi, y)|}{|(2\pi k)^\alpha|}, \quad \forall\alpha \in \mathbb{N}_0^d,\ \forall k, j \in \mathbb{Z}^d_*. \tag{10.2.6}$$

Finally, identity (10.2.4) implies that:

$$\begin{aligned}
\left\|P^\varepsilon_\varphi \Psi^\varepsilon\right\|^2_{H^r_\varepsilon(\mathbb{R}^d, H^s(\mathbb{T}^d))} &= \int_{\mathbb{R}^d} \sum_{k\in\mathbb{Z}^d} \left| c(\varepsilon\xi + 2\pi k)\langle 2\pi k\rangle^s \sum_{j\in\mathbb{Z}^d} c(\varepsilon\xi + 2\pi j)\, \langle\varepsilon\xi\rangle^r\, \hat{\Psi}^\varepsilon_j(\xi)\right|^2 d\xi \\
&\leqslant \int_{\mathbb{R}^d} \sum_{k,j\in\mathbb{Z}^d} \left| c(\varepsilon\xi + 2\pi k)\, c(\varepsilon\xi + 2\pi j)\langle 2\pi k\rangle^s \langle 2\pi j\rangle^s\, \langle\varepsilon\xi\rangle^r\, \hat{\Psi}^\varepsilon_j(\xi)\right|^2 d\xi,
\end{aligned}$$

therefore, it suffices to show that

$$\sup_{\xi\in\mathbb{R}^d}\sum_{k\in\mathbb{Z}^d}|c(\xi+2\pi k)\,c(\xi+2\pi j)\langle 2\pi k\rangle^s|^2\;<\;\infty, \tag{10.2.7}$$

where we have no dependence on ε. This is made by fixing a multi-index $\alpha\in\mathbb{N}_0^d$ with $|\alpha|>d+2s$ and, given any $\xi\in\mathbb{R}^d$, choosing[2] $\eta\in\mathcal{B}=[-2\pi,2\pi]^d$ and $p\in\mathbb{Z}_*^d$ such that $\xi=\eta-2\pi p$. Then, by estimates (10.2.5) and (10.2.6), if follows that, for $k\neq 0$:

$$|c(\eta+2\pi(k-p))\,c(\eta+2\pi(j-p))|^2\;\sim\;\frac{1}{\langle 2\pi k\rangle^{|\alpha|}}\left\|\partial_y^\alpha\varphi\right\|^2_{L^\infty(\mathcal{B}\times\mathbb{T}^d)}\sum_{\substack{\beta\in\mathbb{N}_0^d\\|\beta|\leqslant|\alpha|}}\left\|\partial_y^\beta\varphi\right\|^2_{L^\infty(\mathcal{B}\times\mathbb{T}^d)},$$

which carries (10.2.7) and, consequently, completes the proof. □

Corollary 10.2.4. *Define $\tilde{P}^\varepsilon_{\varphi_n}:H^r_\varepsilon(\mathbb{R}^d)\longrightarrow H^r_\varepsilon\left(\mathbb{R}^d,H^s(\mathbb{T}^d)\right)$ by making $\tilde{P}^\varepsilon_{\varphi_n}\Psi=P^\varepsilon_{\varphi_n}\tilde{\Psi}$, where $\tilde{\Psi}(x,y)=\Psi(x)$. Then, for all $r\geqslant 0$ and $s\geqslant 0$, the operator $\tilde{P}^\varepsilon_{\varphi_n}$ is uniformly bounded with respect to $\varepsilon>0$.*

Proof. Observe that, if $\Psi^\varepsilon\in H^r_\varepsilon(\mathbb{R}^d)$, then for any $s\geqslant 0$ one has $\tilde{\Psi}^\varepsilon\in H^r_\varepsilon\left(\mathbb{R}^d,H^s(\mathbb{T}^d)\right)$, and use Lemma 10.2.3. □

At this point, we should control how the ε-oscillation property behaves with respect to the restriction to the diagonal $y=\frac{x}{\varepsilon}$. To work properly, let us define the operator L^ε that maps a function Q defined on $\mathbb{R}^d\times\mathbb{T}^d$ to $L^\varepsilon Q$ on $\mathbb{R}^d$:

$$L^\varepsilon Q(x)=Q\left(x,\frac{x}{\varepsilon}\right).$$

Lemma 10.2.5. *Suppose $s>d$ and $r\geqslant 0$. Then the operator*

$$L^\varepsilon:H^r_\varepsilon\Big(\mathbb{R}^d,H^s(\mathbb{T}^d)\Big)\longrightarrow L^2(\mathbb{R}^d)$$

is uniformly bounded with respect to ε and, if $(Q^\varepsilon)_{\varepsilon>0}$ in $H^r_\varepsilon\left(\mathbb{R}^d,H^s(\mathbb{T}^d)\right)$ is bounded and satisfies the estimate

$$\limsup_{\varepsilon\to 0}\left\|\,\mathbb{1}_{\{\|\xi\|\geqslant R\}}(\varepsilon\partial_x)\,Q^\varepsilon\,\right\|_{H^r_\varepsilon\left(\mathbb{R}^d,H^s(\mathbb{T}^d)\right)}\underset{R\to\infty}{\longrightarrow}0, \tag{10.2.8}$$

then the family $(L^\varepsilon Q^\varepsilon)_{\varepsilon>0}$ will also be bounded in $L^2(\mathbb{R}^d)$ and ε-oscillating.

Proof. Let be $Q^\varepsilon\in L^2\left(\mathbb{R}^d,H^s(\mathbb{T}^d)\right)$ and calculate, for every $x\in\mathbb{R}^d$ fixed, the Fourier coefficients of $Q^\varepsilon(x,\cdot\,)$:

$$Q^\varepsilon_k(x)=\int_{\mathbb{T}^d}Q^\varepsilon(x,y)e^{-2\pi ik\cdot y}dy\quad\text{and}\quad Q^\varepsilon(x,y)=\sum_{k\in\mathbb{Z}^d}Q^\varepsilon_k(x)e^{2\pi ik\cdot y}. \tag{10.2.9}$$

Of course, the fact that $Q(x,\cdot\,)$ belongs to $H^s(\mathbb{T}^d)$ implies, after a norm estimation, that

$$|\langle\varepsilon\partial_x\rangle^r Q^\varepsilon_k(x)|^2\leqslant\frac{\|\langle\varepsilon\partial_x\rangle^r Q^\varepsilon(x,\cdot\,)\|^2_{H^s(\mathbb{T}^d)}}{\langle 2\pi k\rangle^{2s}},$$

[2]Using $\eta\in\mathcal{B}=[-\pi,\pi)^d$ and $p\in\mathbb{Z}^d$, it is already possible to decompose $\xi=\eta+2\pi p$, in a unique manner, by the way. Here, we used $\mathcal{B}=[-2\pi,2\pi]^d$ for two reasons: to be able to take $p\neq 0$ for any $\xi\in\mathbb{R}^d$, and to have $\mathcal{B}$ compact.

which integrated in x gives

$$\| Q_k^\varepsilon \|_{H_\varepsilon^r(\mathbb{R}^d)} \leqslant \frac{1}{\langle 2\pi k\rangle^s} \| Q^\varepsilon \|_{H_\varepsilon^r\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} . \tag{10.2.10}$$

As a consequence, since $s > d$ and the norm $L^2(\mathbb{R}^d)$ is thinner than $H_\varepsilon^r(\mathbb{R}^d)$ for any $r \geqslant 0$ and $\varepsilon > 0$, there exists a constant $C_s > 0$ such that

$$\|L^\varepsilon Q^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant \sum_{k\in\mathbb{Z}^d} \|Q_k^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant C_s \|Q^\varepsilon\|_{H_\varepsilon^r\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} ,$$

where we have used (10.2.9) in the first and (10.2.10) in the second inequality, proving uniform boundedness for L^ε.

Let us now show that, under condition (10.2.8), $q^\varepsilon = L^\varepsilon Q^\varepsilon$ defines an ε-oscillating family. Start by taking $\delta > 0$; since $s > d$, there exists a $N_\delta > 0$ such that

$$\sum_{\|k\|>N_\delta} \frac{1}{\langle 2\pi k\rangle^s} < \delta;$$

define:

$$q_\delta^\varepsilon(x) = \sum_{\|k\|\leqslant N_\delta} Q_k^\varepsilon(x) e^{2\pi i k\cdot\frac{x}{\varepsilon}}.$$

Clearly, from (10.2.10) we have got

$$\|q^\varepsilon - q_\delta^\varepsilon\|_{L^2(\mathbb{R}^d)} \leqslant \delta \| Q^\varepsilon \|_{H_\varepsilon^r\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} , \tag{10.2.11}$$

therefore, it is enough to show that, for any $\delta > 0$, the collection $(q_\delta^\varepsilon)_{\varepsilon>0}$ is ε-oscillating.

Calculating the Fourier transform of q_δ^ε,

$$\hat{q}_\delta^\varepsilon(\xi) = \sum_{\|k\|\leqslant N_\delta} \hat{Q}_k^\varepsilon \left(\xi - \frac{2\pi k}{\varepsilon}\right) ,$$

we find out that

$$\left\| \mathbb{1}_{\{\|\xi\|\geqslant R\}}(\varepsilon\partial_x)\, q_\delta^\varepsilon \right\|_{L^2(\mathbb{R}^d)} \leqslant \sum_{\|k\|\leqslant N_\delta} \left\| \mathbb{1}_{\{\|\xi\|\geqslant R\}}(\varepsilon\partial_x + 2\pi k)\, Q_k^\varepsilon \right\|_{L^2(\mathbb{R}^d)} . \tag{10.2.12}$$

If $R \gg N_\delta$ is large enough, denote $\tilde{R} = \frac{R}{2}$ and we will have

$$\mathbb{1}_{\{\|\xi\|\geqslant R\}}(\,\cdot\, + 2\pi k) \leqslant \mathbb{1}_{\{\|\xi\|\geqslant \tilde{R}\}}(\,\cdot\,) \qquad \forall\, \|k\| \leqslant N_\delta, \tag{10.2.13}$$

then, putting together (10.2.12), (10.2.13) and (10.2.10) consecutively and recalling that the constant $C_s = \sum_{k\in\mathbb{Z}^d} \frac{1}{\langle 2\pi k\rangle^s}$ is finite, we obtain

$$\begin{aligned} \left\| \mathbb{1}_{\{\|\xi\|\geqslant R\}}(\varepsilon\partial_\varepsilon)\, q_\delta^\varepsilon \right\|_{L^2(\mathbb{R}^d)} &\leqslant \sum_{\|k\|\leqslant N_\delta} \left\| \mathbb{1}_{\{\|\xi\|\geqslant \tilde{R}\}}(\varepsilon\partial_x)\, Q_k^\varepsilon \right\|_{L^2(\mathbb{R}^d)} \\ &\leqslant C_s \left\| \mathbb{1}_{\{\|\xi\|\geqslant \tilde{R}\}}(\varepsilon\partial_x)\, Q^\varepsilon \right\|_{H_\varepsilon^r\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} , \end{aligned}$$

which carries under (10.2.8) and (10.2.11) that

$$\limsup_{\varepsilon\to 0} \left\| \mathbb{1}_{\{\|\xi\|\geqslant R\}}(\varepsilon\partial_x)\, q^\varepsilon \right\|_{L^2(\mathbb{R}^d)} \underset{R\to\infty}{\longrightarrow} \mathcal{O}(\delta).$$

Since we can choose δ arbitrarily small and remembering that $q^\varepsilon = L^\varepsilon Q^\varepsilon$, one concludes that the family $(L^\varepsilon Q^\varepsilon)_{\varepsilon>0}$ is ε-oscillating; its boundedness in $L^2(\mathbb{R}^d)$ is now obvious, since L^ε was proven to be uniformly bounded, and by hypothesis $(Q^\varepsilon)_{\varepsilon>0}$ was a bounded family in $L^2\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$. □

Now, let us prepare the main result for the first ingredient of this chapter's analysis:

Lemma 10.2.6. *If $(\Psi^\varepsilon)_{\varepsilon>0}$ is ε-oscillating and uniformly bounded in $L^2(\mathbb{R}^d)$ with respect to ε, then, for every $n\in\mathbb{N}$, so is the family $(L^\varepsilon P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon)_{\varepsilon>0}$.*

Proof. Fix $r=0$ and $s>d$, recall that $\tilde{P}^\varepsilon_{\varphi_n}\Psi^\varepsilon = P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon$ and that $\tilde{\Psi}^\varepsilon \in L^2(\mathbb{R}^d, H^s(\mathbb{T}^d))$ for any s that we want; uniform boundedness with respect to ε comes from the fact that $\tilde{P}^\varepsilon_{\varphi_n} : L^2(\mathbb{R}^d) \longrightarrow L^2\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$ is uniformly bounded in ε (Corollary 10.2.4), and the same for $L^\varepsilon : L^2\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right) \longrightarrow L^2(\mathbb{R}^d)$ (Lemma 10.2.5).

For ε-oscillation, we will use Lemma 10.2.5 again, but in order to do so one needs to show that $P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon$ satisfies (10.2.8). Let us pass into the frequency space in $\mathbb{R}^d$ and in the torus in order to obtain

$$\left\| \mathbb{1}_{\{\|\xi\|>R\}}(\varepsilon\xi)\, \widehat{P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon}(\xi,\cdot) \right\|^2_{H^s(\mathbb{T}^d)} = \sum_{k\in\mathbb{Z}^d} \left| \langle k\rangle^s\, c_n(\varepsilon\xi + 2\pi k) \int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi, z)}dz\, \mathbb{1}_{\{\|\xi\|>R\}}(\varepsilon\xi)\hat{\Psi}^\varepsilon(\xi) \right|^2,$$

where c_n is given in (10.2.3) for its corresponding φ_n and satisfies (10.2.5) with a multi-index $\alpha \in N_0^d$ such that $|\alpha| > s + \frac{d}{2}$, so as one can find a constant $C_{\alpha,s} > 0$ such that, noting $\mathcal{B} = [-\pi,\pi]^d$ and recalling the periodicity condition (10.2.2):

$$\left\| \mathbb{1}_{\{\|\xi\|>R\}}(\varepsilon\xi)\, \widehat{P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon}(\xi,\cdot) \right\|^2_{H^s(\mathbb{T}^d)} \leqslant C_{\alpha,s} \left\| \varphi_n\, \partial_y^\alpha \varphi_n \right\|^2_{L^\infty(\mathcal{B}\times\mathbb{T}^d)} \left| \mathbb{1}_{\{\|\xi\|>R\}}(\varepsilon\xi)\hat{\Psi}^\varepsilon(\xi) \right|^2,$$

which, after integrating in ξ, implies (10.2.8) for $P^\varepsilon_{\varphi_n}\tilde{\Psi}^\varepsilon$ given that Ψ^ε is ε-oscillating. □

Proposition 10.2.7. *If $(\Psi^\varepsilon)_{\varepsilon>0}$ is ε-oscillating and uniformly bounded in $L^2(\mathbb{R}^d)$ with respect to ε, then, for every $j\in\mathbb{N}$, so is the family $\left(L^\varepsilon \Pi^\varepsilon_{\lambda_j}\tilde{\Psi}^\varepsilon\right)_{\varepsilon>0}$.*

Proof. Obvious, for $\Pi^\varepsilon_{\lambda_j}$ is the finite sum of $P^\varepsilon_{\varphi_n}$ where $P(\xi)\varphi_n(\xi,\cdot) = \lambda_j(\xi)\varphi_n(\xi,\cdot)$. □

10.2.2 Some *a priori* estimates

We now present some *a priori* estimates for the solutions of equation (8.2.2) that will be useful in the proof of Theorem 8.4.2.

Lemma 10.2.8. *Given $s\geqslant 0$, any solution U^ε to (8.2.2) with initial datum $U_0^\varepsilon \in L^2\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$ must satisfy*

$$\|U_t^\varepsilon\|_{H^s_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} \lesssim \|U_0^\varepsilon\|_{H^s_\varepsilon\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)} + \mathcal{O}\left(\varepsilon|t|\right) \tag{10.2.14}$$

for every $t\in R$.

Remark 10.2.9. The lemma is not supposing U_0^ε bounded in $H_\varepsilon^s\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$; this may not hold, and then we will have no estimation for U_t^ε with this norm. The point is that, if U_0^ε is $H_\varepsilon^{2s}\left(\mathbb{R}^d, H^{4s}(\mathbb{T}^d)\right)$ bounded (which will be the case here for $0 \leqslant 2s \leqslant r$ for some $r > 2d$ (as we had assumed in **H0'**)), then the same for U_t^ε in $H^{2s}\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$.

Proof. The spectrum of $P(\varepsilon\partial_x)$ is lower bounded uniformly with respect to ε by the finite constant $M = \inf_{\xi\in[-\pi,\pi]^d\subset\mathbb{R}^d} \lambda_1(\xi)$, hence $P(\varepsilon\partial_x) + |M| + 1 > 0$ uniformly in $\varepsilon > 0$ and, consequently,

$$\tilde{P}(\varepsilon\partial_x) = (P(\varepsilon\partial_x) + |M| + 1)^s$$

will be a fair pseudodifferential operator on the functions of $x \in \mathbb{R}^d$ with smooth, though unbounded symbol. Therefore, it is sufficient to prove that $U_t^{\varepsilon,s} = \tilde{P}(\varepsilon\partial_x)U_t^\varepsilon$ verifies an estimate of the form

$$\|U_t^{\varepsilon,s}\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \leqslant \|U_0^{\varepsilon,s}\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} + \mathcal{O}\left(\varepsilon|t|\right) \tag{10.2.15}$$

and then use Remark 10.2.2 to recover the thinner and thicker norms $H_\varepsilon^s\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$ and $H_\varepsilon^s\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$.

In order to obtain (10.2.15), apply $\tilde{P}(\varepsilon\partial_x)$ to both sides of (8.2.2),

$$i\varepsilon^2\partial_t U_t^{\varepsilon,s} = P(\varepsilon\partial_x)U_t^{\varepsilon,s} + \varepsilon^2 V U_t^{\varepsilon,s} + \varepsilon^2\left[\tilde{P}(\varepsilon\partial_x), V\right]U_t^\varepsilon,$$

and now use a standard energy estimation as we did long ago in Proposition 6.1.2 to get

$$\|U_t^{\varepsilon,s}\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \leqslant \|U_0^{\varepsilon,s}\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} + \int_0^t \left\| \left[\tilde{P}(\varepsilon\partial_x), V\right]U_t^\varepsilon \right\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} ds.$$

It happens that the operator

$$\left[\tilde{P}(\varepsilon\partial_x), V\right] : L^2\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right) \longrightarrow L^2(\mathbb{R}^d\times\mathbb{T}^d)$$

is bounded with norm of order ε, since the commutator with V gives, from (2.1.4), a bounded pseudodifferential operator of order ε on the part depending on x, and it has norm of order 1 onto functions in y, since it corresponds to derivatives of order $2s$ thereon. Consequently:

$$\begin{aligned}\left\| \left[\tilde{P}(\varepsilon\partial_x), V\right]U_t^\varepsilon \right\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} &\leqslant \left\|\left[\tilde{P}(\varepsilon\partial_x), V\right]\right\|_{\mathcal{B}(L^2(\mathbb{R}^d,H^{2s}(\mathbb{T}^d)),L^2(\mathbb{R}^d\times\mathbb{T}^d))} \|U_t^\varepsilon\|_{L^2(\mathbb{R}^d,H^{2s}(\mathbb{T}^d))} \\ &\lesssim \varepsilon\,\|U_0^\varepsilon\|_{L^2(\mathbb{R}^d,H^{2s}(\mathbb{T}^d))},\end{aligned}$$

where the identity $\|U_t^\varepsilon\|_{L^2\left(\mathbb{R}^d,H^{2s}(\mathbb{T}^d)\right)} = \|U_0^\varepsilon\|_{L^2\left(\mathbb{R}^d,H^{2s}(\mathbb{T}^d)\right)}$ comes from multiplying (8.2.2) by $\langle\partial_y\rangle^{2s}$ and doing the very same estimate as above.

Hence, if $\|U_0^\varepsilon\|_{H_\varepsilon^s\left(\mathbb{R}^d,H^{2s}(\mathbb{T}^d)\right)}$ is finite, then so is $\|U_0^{\varepsilon,s}\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}$ and the lemma is proven. If not, then $\|U_0^\varepsilon\|_{H_\varepsilon^s\left(\mathbb{R}^d,H^{2s}(\mathbb{T}^d)\right)}$ is infinite and (10.2.14) is trivially satisfied. □

Finally, we are able to understand how strongly ε-oscillating sequences entails good convergence properties concerning the Bloch decomposition. Next step is to understand how strongly the Bloch series converges, and to reduce its analysis to that of a finite superposition of Bloch waves. The content of the following lemma will be useful for these two aims.

Lemma 10.2.10. *Let be $s \geqslant 0$ and suppose that the family $(\Psi^\varepsilon)_{\varepsilon>0}$ is uniformly bounded in $H^{2s}_\varepsilon\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$. It follows that:*

$$\limsup_{\varepsilon\to 0} \sum_{n>N} \left\|P^\varepsilon_{\varphi_n}\Psi^\varepsilon\right\|^2_{H^s_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} \underset{N\to\infty}{\longrightarrow} 0.$$

Proof. To begin with, the norms in the equation above are well-defined, for as we have seen in Lemma 10.2.3, $P^\varepsilon_{\varphi_n}$ is bounded onto $H^s_\varepsilon\left(\mathbb{R}^d, H^s(T^d)\right)$. This enables us to use Remark 10.2.2 and state:

$$\left\|P^\varepsilon_{\varphi_n}\Psi^\varepsilon\right\|_{H^s_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} \lesssim \left\|P(\varepsilon\partial_x)^s P^\varepsilon_{\varphi_n}\Psi^\varepsilon\right\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}.$$

Now, recall that

$$\widehat{P^\varepsilon_{\varphi_n}\Psi^\varepsilon}(\xi, y) = \varphi_n(\varepsilon\xi, y)\int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi, z)}\,\hat{\Psi}^\varepsilon(\xi, y)\,dz$$

and that

$$P(\varepsilon\xi)^s\,\widehat{P^\varepsilon_{\varphi_n}\Psi^\varepsilon}(\xi, y) = \lambda^s_n(\varepsilon\xi)\,\varphi_n(\varepsilon\xi, y)\int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi, z)}\,\hat{\Psi}^\varepsilon(\xi, z)\,dz.$$

Observe further that one has

$$\begin{aligned}\sum_{n\in\mathbb{N}} \left|\lambda^s_n(\varepsilon\xi)\int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi, z)}\,\hat{\Psi}^\varepsilon(\xi, z)dz\right|^2 &= \left\|P(\varepsilon\xi)^s\,\hat{\Psi}^\varepsilon(\xi,\cdot)\right\|^2_{L^2(\mathbb{T}^d)}\\ &\leqslant \mathfrak{p}_{4s}(\varepsilon\xi)\left\|\hat{\Psi}^\varepsilon(\xi,\cdot)\right\|^2_{H^{2k}(\mathbb{T}^d)},\end{aligned}$$

where $\mathfrak{p}_{4s}(\xi) = \|P^s(\xi)\|^2_{\mathcal{B}(H^{2s}(\mathbb{T}^d), L^2(\mathbb{T}^d))}$ is a non-negative polynomial of degree at most $4s$, since, for each ξ, $P(\xi)$ consists of derivatives in y of order at most $2s$, and, therefore, its norm on $H^{2s}(\mathbb{T}^d)$ into $L^2(\mathbb{T}^d)$ is of order 1. Consequently, there exists $C > 0$ independent of ε such that:

$$\begin{aligned}\sum_{n\in\mathbb{N}} \left\|P^\varepsilon_{\varphi_n}\Psi^\varepsilon\right\|^2_{H^s_\varepsilon\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)} &\lesssim \sum_{n\in\mathbb{N}}\int_{\mathbb{R}^d}\left|\lambda^s_n(\varepsilon\xi)\int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\xi, z)}\,\hat{\Psi}^\varepsilon(\xi, z)dz\right|^2\\ &\leqslant \int_{\mathbb{R}^d}\mathfrak{p}_{4s}(\varepsilon\xi)\left\|\hat{\Psi}^\varepsilon(\xi,\cdot)\right\|^2_{H^{2s}(\mathbb{T}^d)}\\ &\lesssim \|\Psi^\varepsilon\|^2_{H^{2s}_\varepsilon\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)}\\ &\leqslant C.\end{aligned}$$

In other words, we have an absolutely convergent series $\sum_{j\in\mathbb{N}}|c^\varepsilon_j|^2 \leqslant C < \infty$ uniformly bounded with respect to ε. Let us show that

$$\lim_{N\to\infty}\limsup_{\varepsilon\to 0}\sum_{j>N}|c^\varepsilon_j|^2 = 0. \tag{10.2.16}$$

Supposing that (10.2.16) is false, then there exists $\delta > 0$ for which one can find an increasing sequence of $N > 0$ and sequences $(\varepsilon_k(N))_{k\in\mathbb{N}}$ converging to 0 such that, for any $k \in \mathbb{N}$,

$$\sum_{j>N}\left|c^{\varepsilon_k(N)}_j\right|^2 > \delta. \tag{10.2.17}$$

Now, define a new sequence $(\tilde{\varepsilon}_k)_{k\in\mathbb{N}}$ as:

$$\begin{aligned}&\tilde{\varepsilon}_1 = \varepsilon_1(1)\\ &\tilde{\varepsilon}_k = \varepsilon_{k^*}(k), \quad \text{with } k^* = \min\{j \in \mathbb{N} : \varepsilon_j(k) < \tilde{\varepsilon}_{k-1}\},\end{aligned}$$

which is of course converging to 0, and define $s_k = \sum_{j\leqslant k} \left| c_j^{\tilde{\varepsilon}_k} \right|^2$, which is a bounded sequence, for $s_k \leqslant \sup_{\varepsilon>0} \sum_{j\in\mathbb{N}} |c_j^\varepsilon|^2 \leqslant C$. Therefore,

$$\limsup_{N\to\infty} \sum_{j\leqslant N} \left| c_j^{\tilde{\varepsilon}_N} \right|^2 \leqslant C,$$

which in any case implies

$$\sum_{j>N} \left| c_j^{\tilde{\varepsilon}_N} \right|^2 \underset{R\to\infty}{\longrightarrow} 0,$$

allowing us to find $N_0 > 0$ and $k_0 \in \mathbb{N}$ such that

$$\sum_{j>N_0} \left| c_j^{\varepsilon_{k_0}(N_0)} \right|^2 < \delta$$

will be in contradiction with (10.2.17)!

This proves (10.2.16); now just take $c_n^\varepsilon = \left\| P_{\varphi_n}^\varepsilon \Psi^\varepsilon \right\|_{H_\varepsilon^s\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)}$. □

Let us now resume the analysis of our concrete initial data $(\psi_0^\varepsilon)_{\varepsilon>0}$, which are supposed strongly ε-oscillating of order at least r for some $r > 2d$, as required Theorem 8.4.2 (and therefore ε-oscillating of order 0 and uniformly bounded in $L^2(\mathbb{R}^d)$). Denote by U^ε the solutions of (8.2.2) whose initial data are $U_0^\varepsilon = \tilde{\psi}_0^\varepsilon$, with $\tilde{\psi}_0^\varepsilon(x, y) = \psi_0^\varepsilon(x)$. Clearly, for every $0 \leqslant 2s \leqslant r$, U_0^ε are uniformly bounded in $H_\varepsilon^{2s}\left(\mathbb{R}^d, H^{4s}(\mathbb{T}^d)\right)$ and, from Lemma 10.2.8, so are U_t^ε, $t \in \mathbb{R}$, in $H_\varepsilon^{2s}\left(\mathbb{R}^d, H^{2s}(\mathbb{T}^d)\right)$.

In equation (8.2.4) in the introduction in Chapter 8, we wrote U^ε as a formal series with terms given in (8.2.5), which we called the Bloch decomposition. Let us now make this statement concrete and specify in which sense this series' convergence is to be understood.

Proposition 10.2.11. *For every $0 \leqslant s \leqslant \frac{r}{2}$, $t \in \mathbb{R}$ and U^ε as described above, the Bloch decomposition series*

$$U_t^\varepsilon = \sum_{j\in\mathbb{N}} \Pi_{\lambda_j}^\varepsilon U_t^\varepsilon$$

converges in the norm $H_\varepsilon^s\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right)$.

Proof. Recalling that $\Pi_{\lambda_j}^\varepsilon$ is a finite sum of $P_{\varphi_n}^\varepsilon$ for which φ_n have eigenvalue λ_j, check with Lemma 10.2.8 that U_t^ε are uniformly bounded in $H_\varepsilon^{2s}(\mathbb{R}^d, H^{2s}(\mathbb{T}^d))$ and just apply Lemma 10.2.10. □

By unicity, the solution ψ^ε of (8.1.2) whose initial datum is ψ_0^ε must satisfy, for any $t \in \mathbb{R}$,

$$\psi_t^\varepsilon = L^\varepsilon U_t^\varepsilon;$$

therefore, given that $L^\varepsilon : H_\varepsilon^s\left(\mathbb{R}^d, H^s(\mathbb{T}^d)\right) \longrightarrow L^2(\mathbb{R}^d)$ is bounded for $s > d$ (Lemma 10.2.5), for each $t \in \mathbb{R}$,

$$\psi_t^\varepsilon = \sum_{j\in\mathbb{N}} \psi_{j,t}^\varepsilon \tag{10.2.18}$$

converges in $L^2(\mathbb{R}^d)$, where

$$\psi^\varepsilon_{j,t} = L^\varepsilon \Pi^\varepsilon_{\lambda_j} U^\varepsilon_t.$$

From Propositon 10.2.7, the family $(\psi^\varepsilon_{j,0})_{\varepsilon>0}$ is ε-oscillating and bounded in $L^2(\mathbb{R})$. Concerning its evolution:

Lemma 10.2.12. *For every $j \in \mathbb{N}$, ψ^ε_j solves an equation of the form:*

$$\left\{ \begin{array}{l} i\varepsilon^2 \partial_t \psi^\varepsilon_j(t,x) = \lambda_j(\varepsilon\partial_x)\psi^\varepsilon_j(t,x) + \varepsilon^2 V(x)\psi^\varepsilon_j(t,x) + \varepsilon^3 g^\varepsilon_j(t,x) \\ \psi^\varepsilon_j(0,\cdot) = L^\varepsilon \Pi^\varepsilon_{\lambda_j} \tilde{\psi}^\varepsilon_0, \end{array} \right. \tag{10.2.19}$$

where there exists $C > 0$ such that $\left\| g^\varepsilon_j(t,\cdot) \right\|_{L^2(\mathbb{R}^d)} \leqslant C$ locally uniformly in t. Besides, $(\psi^\varepsilon_{j,t})_{\varepsilon>0}$ is ε-oscillating and uniformly bounded with respect to ε.

Proof. In order to simplify the notation, we shall assume that the Bloch eigenvalues λ_n are simple. The proof in the general case is a straightforward modification of the one we present below. Define

$$u^\varepsilon_n(t,x) = \int_{\mathbb{T}^d} \overline{\varphi_n(\varepsilon\partial_x, y)} U^\varepsilon(t,x,y)dy \quad \text{and} \quad \psi^\varepsilon_n(t,\cdot) = L^\varepsilon \varphi_n(\varepsilon\partial_x, y)\, u^\varepsilon_n(t,\cdot).$$

We start by applying $\overline{\varphi_n(\varepsilon\partial_x, y)}$ to both sides of (8.2.2) and integrating in the torus, which gives

$$i\varepsilon^2 \partial_t u^\varepsilon_n(t,x) = \lambda_n(\varepsilon\partial_x)u^\varepsilon_n(t,x) + \varepsilon^2 V(x) u^\varepsilon_n(t,x) + \varepsilon^3 f^\varepsilon_n(t,x),$$

where

$$f^\varepsilon_n(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{T}^d} \left[\overline{\varphi_n(\varepsilon\partial_x, y)}, V(x) \right] U^\varepsilon(t,x,y)dy;$$

now we apply $L^\varepsilon \varphi(\varepsilon\partial_x, y)$:

$$i\varepsilon^2 \partial_t \psi^\varepsilon_n(t,x) = \lambda_n(\varepsilon\partial_x)\psi^\varepsilon_n(t,x) + \varepsilon^2 V(x)\psi^\varepsilon_n(t,x) + \varepsilon^3 g^\varepsilon_n(t,x) + h^\varepsilon_n(t,x),$$

with

$$g^\varepsilon_n(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{T}^d} \left[\varphi_n\left(\varepsilon\partial_x, \frac{x}{\varepsilon}\right) \overline{\varphi_n(\varepsilon\partial_x, y)}, V(x) \right] U^\varepsilon(t,x,y)dy$$

and

$$h^\varepsilon_n(t,x) = \left[L^\varepsilon \varphi_n(\varepsilon\partial_x, y), \lambda_n(\varepsilon\partial_x) \right] u^\varepsilon_n(t,x).$$

Since λ_n is $2\pi\mathbb{Z}^d$-periodic, it is easy to show that $h^\varepsilon_n = 0$:

$$\begin{aligned} L^\varepsilon \varphi_n(\varepsilon\partial_x, y)\lambda_n(\varepsilon\partial_x) &= \sum_{k,k' \in \mathbb{Z}^d} e^{2\pi i k \cdot \frac{x}{\varepsilon}} c^k_n(\varepsilon\partial_x) e^{-ik' \cdot (i\partial_x)} d^{k'}_n \\ &= \sum_{k,k' \in \mathbb{Z}^d} e^{-ik' \cdot (2\pi k + i\partial_x)} d^{k'}_n e^{2\pi i k \cdot \frac{x}{\varepsilon}} c^k_n(\varepsilon\partial_x) \\ &= \lambda_n(\varepsilon\partial_x) L^\varepsilon \varphi_n(\varepsilon\partial_x, y), \end{aligned}$$

where c^k_n and $d^{k'}_n$ are suitable Fourier coefficients; moreover, symbolic calculus for semiclassical pseudodifferential operators together with the uniform boundedness of U^ε_t for compact times, estimated in Lemma 10.2.8, implies that there exists $C > 0$ such that:

$$\| f^\varepsilon_n(t,\cdot) \|_{L^2(\mathbb{R}^d)} \leqslant C \quad \text{and} \quad \| g^\varepsilon_n(t,\cdot) \|_{L^2(\mathbb{R}^d)} \leqslant C$$

locally uniformly in $t \in \mathbb{R}$, which proves either Proposition 8.2.2 in Chapter 8 and equation (10.2.19) above.

Uniform boundedness in ε for $\psi^\varepsilon_{j,t}$ comes from either the equation or, alternatively, from Proposition 10.2.7 and the uniform boundedness of U^ε_t; however, this proposition does not automatically gives ε-oscillation for $\psi^\varepsilon_{j,t}$ for $t \neq 0$, so we need to show it directly from (10.2.19) by taking an appropriate cut-off $\chi \in C_0^\infty(\mathbb{R}^d)$ such that $\chi(\xi) = 0$ for $\|\xi\| > 1$, $\chi \leqslant 1$, and applying $\left(1 - \chi\left(\frac{\varepsilon\partial_x}{R}\right)\right)$ to this equation in order to obtain, after an energy estimation:

$$\limsup_{\varepsilon\to 0} \left\| \left(1 - \chi\left(\frac{\varepsilon\partial_x}{R}\right)\right) \psi^\varepsilon_{j,t} \right\|_{L^2(\mathbb{R})} \leqslant \limsup_{\varepsilon\to 0} \left\| \left(1 - \chi\left(\frac{\varepsilon\partial_x}{R}\right)\right) \psi^\varepsilon_{j,0} \right\|_{L^2(\mathbb{R})},$$

which eventually gives the aimed result letting $R \longrightarrow \infty$ and taking into account that the initial data $\psi^\varepsilon_{j,0}$ are ε-oscillating. □

10.2.3 Wigner measures of ψ^ε and the adherence of $|\psi^\varepsilon|^2$

The first result below describes the Wigner measure of a family of solutions to (8.1.2) by means of the semiclassical measures linked to the terms in the Bloch decomposition.

Lemma 10.2.13. *Let* $(\psi^\varepsilon)_{\varepsilon>0}$ *be a sequence of solutions to* (8.1.2) *issued from ε-oscillating initial data satisfying* (8.4.4) *in **H0'**. Then there exists* $(\varepsilon_k)_{k\in\mathbb{N}}$ *such that, for every* $\phi \in C_0^\infty(\mathbb{R})$ *and* $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$*:*

$$\lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi^{\varepsilon_k}, \phi\psi^{\varepsilon_k}\right\rangle_{L^2(\mathbb{R}^{d+1})} = \sum_{j\in I} \int_{\mathbb{R}\times\mathbb{R}^{2d}} a(t, \lambda_j(\xi), x, \xi)|\phi(t)|^2 \mu_j(dt, dx, d\xi),$$

where, for each $j \in I$, the measures μ_j on $\mathbb{R} \times \mathbb{R}^{2d}$ are supported on

$$\Lambda_j = \left\{(t, x, \xi) \in \mathbb{R} \times \mathbb{R}^{2d} : \nabla\lambda_j(\xi) = 0\right\}$$

and, for every $b \in C_0^\infty(\mathbb{R} \times \mathbb{R}^{2d})$:

$$\lim_{k\to\infty} \int_{\mathbb{R}} \left\langle \mathrm{op}_{\varepsilon_k}(b)\psi_j^{\varepsilon_k}, \psi_j^{\varepsilon_k}\right\rangle dt = \int_{\mathbb{R}\times\mathbb{R}^{2d}} b(t, x, \xi)\mu_j(dt, dx, d\xi),$$

as usual in standard semiclassical analysis.

Proof. We apply Proposition 10.1.2 to obtain $(\varepsilon_k)_{k\in\mathbb{N}}$ such that, for every $\phi \in C_0^\infty(\mathbb{R})$ and $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$:

$$\lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi^{\varepsilon_k}, \phi\psi^{\varepsilon_k}\right\rangle_{L^2(\mathbb{R}^{d+1})} = \int_{\mathbb{R}^{2(d+1)}} a(t, \tau, x, \xi)|\phi(t)|^2 \widetilde{\mu}(dt, d\tau, dx, d\xi)$$

for some positive measure $\widetilde{\mu}$ on $\mathbb{R}^{2(d+1)}$. From (8.4.4) one also has:

$$\left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi^{\varepsilon_k}, \phi\psi^{\varepsilon_k}\right\rangle_{L^2(\mathbb{R}^{d+1})} = \sum_{j,l\in I} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi_j^{\varepsilon_k}, \phi\psi_l^{\varepsilon_k}\right\rangle_{L^2(\mathbb{R}^{d+1})} + o(\varepsilon). \tag{10.2.20}$$

Lemma 10.2.14. *The following holds:*

1. *if $j \neq l$, then for all $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$,*

$$\lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi_j^{\varepsilon_k}, \phi\psi_l^{\varepsilon_k}\right\rangle_{L^2(\mathbb{R}^{d+1})} = 0;$$

2. *if* $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$ *is such that* $a(t,\tau,x,\xi) = 0$ *in a neighbourhood of* $\{\tau = \lambda_j(\xi)\}$, *then*

$$\lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi_j^{\varepsilon_k}, \phi\psi_j^{\varepsilon_k} \right\rangle_{L^2(\mathbb{R}^{d+1})} = 0.$$

Before proving Lemma 10.2.14, we will show how the result follows from it. Let us denote

$$D_j = \left\{ (\tau,\xi) \in \mathbb{R}^{d+1} : \tau = \lambda_j(\xi) \right\}.$$

Remark 10.2.15. Notice that if τ is restricted to a compact of $\mathbb{R}$, then there exists a finite number of eigenvalues $\lambda_j(\xi)$ such that $\tau = \lambda_j(\xi)$, since the Bloch energies are supposed well separate in **H0'** (in the sense of (8.4.3)).

So, let be $j \in \mathbb{N}$; the separation between the eigenvalues λ_j allows one to find an open neighbourhood U_j of D_j such that $U_j \cap D_l = \emptyset$ for every $l \in \mathbb{N}$ with $j \neq l$. Take $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$ such that $a(t,\tau,x,\xi) = 0$ if $(\tau,\xi) \notin U_j$; (10.2.20) together with the lemma implies:

$$\lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi^{\varepsilon_k}, \phi\psi^{\varepsilon_k} \right\rangle_{L^2(\mathbb{R}^{d+1})} = \lim_{k\to\infty} \left\langle \mathrm{op}_{\varepsilon_k}(a^{\varepsilon_k})\phi\psi_j^{\varepsilon_k}, \phi\psi_j^{\varepsilon_k} \right\rangle_{L^2(\mathbb{R}^{d+1})}.$$

Thus, Propositions 10.1.2 and 10.1.3 combined give, after a diagonal extraction for obtaining a suitable subsequence $(\varepsilon_{k_{k'}})_{k'\in\mathbb{N}}$ and after taking the semiclassical limit:

$$\int_{\mathbb{R}^{2(d+1)}} a(t,\tau,x,\xi)|\phi(t)|^2 \widetilde{\mu}(dt,d\tau,dx,d\xi) = \int_{\mathbb{R}\times\mathbb{R}^{2d}} a(t,\lambda_n(\xi),x,\xi)|\phi(t)|^2 \mu_j(dt,dx,d\xi),$$

where μ_j is a Wigner measure for ψ_j^ε, which is moreover supported over the set of critical points of λ_j. This affirmation comes from the fact that the functions ψ_j^ε obey to equation (10.2.19) in Lemma 10.2.12, so as Proposition 9.1.1 applies.

If $a \in C_0^\infty(\mathbb{R}^{2(d+1)})$ is arbitrary, one covers its support with a finite (Remark 10.2.15) union of open neighbourhoods U_j of D_j such that $U_j \cap D_l = \emptyset$ for all $l \neq j$ and decomposes a as a sum of functions supported on each U_j. The result then follows from the previous computation. □

Proof of Lemma 10.2.14. Claim 2 follows directly from Proposition 10.1.3. So does claim 1, but with some more work. Indeed, consider the distribution

$$\left\langle \widetilde{W}_{j,l}^\varepsilon, a \right\rangle_{\mathbb{R}^{2(d+1)}} = \left\langle \mathrm{op}_{\varepsilon_k}(a^\varepsilon)\phi\psi_j^\varepsilon, \phi\psi_l^\varepsilon \right\rangle_{L^2(\mathbb{R}^{d+1})},$$

where $j \neq n$. Analogously to what we have done in equation (6.2.3), Chapter 6, Section 6.2, with some symbolic calculus one sees that it converges to an interference term between the measures of ψ_j^ε and ψ_l^ε and, therefore, its support is included in the intersection of the supports of $\widetilde{\mu}_j$ and $\widetilde{\mu}_l$, which the proposition shows to be disjoint. □

It is important to observe that, although $I \subset \mathbb{N}$ is in general infinite, the sum in Lemma 10.2.13 is in practice always over a finite subset of I, since there we are taking time-localized test functions that are compactly supported in the variable τ and, as we have discussed in Remark 10.2.15, there may only be a finite number of λ_j such that $a(t,\lambda_j(\xi),x,\xi) \neq 0$, which carries that for all but a finite number of indices $j \in I$ we are summing zeros.

If we are to extend our analysis to the current test functions in $C_0^\infty(\mathbb{R}_t \times \mathbb{R}^{2d}_{x,\xi})$, that necessarily do not have compact support in τ, or even more, to symbols not depending on

ξ (as it is the case in Theorems 8.4.2 and 8.4.3), we need to project $\widetilde{\mu}$ integrating it with respect to τ and, eventually, to ξ as well, and here is where ε-oscillation (of order 0) will be required.

Lemma 10.2.16. *If ψ_j^ε solves* (10.2.19) *and, for every $t \in \mathbb{R}$, $(\psi_{j,t}^\varepsilon)_{\varepsilon>0}$ is ε-oscillating, then* (10.1.4) *holds for $(\phi\psi_j^\varepsilon)_{\varepsilon>0}$ with any $\phi \in C_0^\infty(\mathbb{R})$.*

Proof. Let be $\phi \in C_0^\infty(\mathbb{R})$ and choose a cut-off $\chi \in C_0^\infty(\mathbb{R})$ with $\chi(\tau) = 1$ for $|\tau| \leqslant 1$, $\chi(\tau) = 0$ for $|\tau| > 2$ and $\chi \leqslant 1$. Let be $B \in C^\infty(\mathbb{R})$ such that $1 - \chi(\tau) = \tau B(\tau)$. We have:

$$(1-\chi)\left(\varepsilon^2\partial_t - \lambda_j(\varepsilon\partial_x)\right)(\phi u^\varepsilon) = \varepsilon^2 B\left(\varepsilon^2\partial_t - \lambda_j(\varepsilon\partial_x)\right)\left(V(x)\phi u^\varepsilon + \tilde{g}^\varepsilon\right),$$

with $\tilde{g}^\varepsilon$ uniformly bounded in $L^2(\mathbb{R}_t \times \mathbb{R}_x^d)$. As a consequence,

$$\phi u^\varepsilon = \chi\left(\varepsilon^2\partial_t - \lambda_j(\varepsilon\partial_x)\right)(\phi u^\varepsilon) + \varepsilon^2 r^\varepsilon, \tag{10.2.21}$$

with $\mathrm{op}_\varepsilon(a) r^\varepsilon$ uniformly bounded in $L^2(\mathbb{R}_t \times \mathbb{R}_x^d)$ for any $a \in C_0^\infty(\mathbb{R}_{x,\xi}^{2d})$. Besides, using that u_t^ε is ε-oscillating for all $t \in \mathbb{R}$, we can write, for $R, c > 0$,

$$(1-\chi)\left(\frac{1}{R}\left(|\varepsilon^2\partial_t| + \|\varepsilon\partial_x\|\right)\right)(\phi u^\varepsilon) = (1-\chi)\left(\frac{1}{R}\left(|\varepsilon^2\partial_t| + \|\varepsilon\partial_x\|\right)\right)\chi\left(\frac{\varepsilon\|\partial_x\|}{cR}\right)(\phi u^\varepsilon) + \theta_{\varepsilon,R},$$

where

$$\limsup_{\varepsilon\to 0}\|\theta_{\varepsilon,R}\|_{L^2(\mathbb{R}_t\times\mathbb{R}_x^d)} \underset{R\to\infty}{\longrightarrow} 0.$$

Therefore, using (10.2.21), we obtain in $L^2(\mathbb{R}_t \times \mathbb{R}_x^d)$:

$$\begin{aligned}&(1-\chi)\left(\frac{1}{R}\left(|\varepsilon^2\partial_t| + \|\varepsilon D_x\|\right)\right)(\phi u^\varepsilon)\\ &= (1-\chi)\left(\frac{1}{R}\left(|\varepsilon^2\partial_t| + \|\varepsilon\partial_x\|\right)\right)\chi\left(\frac{\varepsilon\|\partial_x\|}{cR}\right)\chi\left(\varepsilon^2\partial_t - \lambda_j(\varepsilon\partial_x)\right)(\phi u^\varepsilon) + \theta_{\varepsilon,R} + \mathcal{O}(\varepsilon^2).\end{aligned}$$

Let $M > 0$ such that, for all $\xi \in \mathbb{R}^d$,

$$|\lambda_j(\xi)| \le M(1 + \|\xi\|);$$

to conclude the proof, observe that choosing $R > 2(2+M)$ and $c(M+1) < \frac{1}{4}$, then the support of

$$(\tau,\xi) \longmapsto (1-\chi)\left(\frac{|\tau| + \|\xi\|}{R}\right)\chi\left(\frac{\|\xi\|}{cR}\right)\chi\left(\tau - \lambda_j(\xi)\right)$$

is empty. □

Next result shows how the Wigner measures can be used to obtain the limits of the position densities $|\psi^\varepsilon|^2$.

Proposition 10.2.17. *Let $(\psi^\varepsilon)_{\varepsilon>0}$ be a family of solutions to* (8.1.2) *issued from strongly ε-oscillating initial data of order $r > 2d$. Let $(\varepsilon_k)_{k\in\mathbb{N}}$ and μ_j be as in Lemma* (10.2.13)*, and suppose that $(|\psi^{\varepsilon_k}|^2)_{k\in\mathbb{N}}$ converges to a measure γ on $\mathbb{R}\times\mathbb{R}^d$. Then, for any $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$, one has:*

$$\int_{\mathbb{R}\times\mathbb{R}^d}\phi(t,x)\gamma(dt,dx) = \sum_{j\in I}\int_{\mathbb{R}\times\mathbb{R}^{2d}}\phi(t,x)\mu_j(dt,dx,d\xi).$$

Proof. Set $U_0^\varepsilon = \tilde{\psi}_0^\varepsilon$ and U^ε the corresponding solution to (8.2.2). Decompose:

$$U^\varepsilon = U_N^\varepsilon + R_N^\varepsilon \quad \text{with} \quad U_N^\varepsilon = \sum_{j=1}^{N} \Pi_{\lambda_j}^\varepsilon U^\varepsilon.$$

Write:

$$\psi^\varepsilon = g_N^\varepsilon + r_N^\varepsilon \quad \text{with} \quad \begin{array}{l} g_N^\varepsilon = L^\varepsilon U_N^\varepsilon = \sum_{n=1}^N \psi_n^\varepsilon \\ r_N^\varepsilon = L^\varepsilon R_N^\varepsilon. \end{array}$$

Lemmata 10.2.10 and 10.2.8 implied that, for each $t \in \mathbb{R}$ and some $r > 2d$,

$$\limsup_{\varepsilon\to 0} \|R_N^\varepsilon(t,\cdot)\|_{H_\varepsilon^r(\mathbb{R}^d, H^r(\mathbb{T}^d))} \underset{N\to\infty}{\longrightarrow} 0,$$

and, for by Lemma 10.2.5 L^ε is continuous from $H_\varepsilon^r\left(\mathbb{R}^d, H^r(\mathbb{T}^d)\right)$ into $L^2(\mathbb{R}^d)$, we had got:

$$\limsup_{\varepsilon\to 0} \|r_N^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \underset{N\to\infty}{\longrightarrow} 0$$

locally uniformly in t, which for compact times lefts us with the analysis of g_N^ε, a finite sum.

Thus, since for each $t \in \mathbb{R}$ $\psi_{j,t}^\varepsilon$ are ε-oscillating (Lemma 10.2.12), Lemma 10.2.16 allows us to apply Proposition 10.1.2 and, therefore, from Lemma 10.2.13 one gets

$$\lim_{k\to\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|g_N^{\varepsilon_k}(t,x)|^2 dxdt \;=\; \sum_{\substack{j\in I\\ j\leqslant N}} \int_{\mathbb{R}\times\mathbb{R}^{2d}} \phi(t,x)\mu_j(dtdx,d\xi),$$

which implies:

$$\lim_{k\to\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(t,x)|\psi^{\varepsilon_k}(t,x)|^2 dxdt \;=\; \lim_{N\to\infty} \sum_{\substack{j\in I\\ j\leqslant N}} \int_{\mathbb{R}\times\mathbb{R}^{2d}} \phi(t,x)\mu_j(dt,dx,d\xi).$$

This is what says the proposition. □

Remark 10.2.18. At the end, strong ε-oscillation on Ψ^ε was needed only to reduce the analysis of an infinite series of Bloch waves to a finite superposition of them, by showing above that its remainder with respect to the whole series does not add much mass to the total sum. In particular, in Proposition 10.2.7 we needed solely normal ε-oscillation on Ψ^ε to make sure this property is transmitted to the terms $P_{\varphi_n}^\varepsilon \tilde{\Psi}^\varepsilon$, so we could drop hypothesis **H0'** and keep solely **H0** in Theorems 8.4.2 and 8.4.3 provided that the initial data ψ_0^ε consist of a finite superposition of Bloch waves with constant multiplicity.

10.3 The main result

At this point, Theorems 8.4.2 and 8.4.3 are basically proven, we just need to bring together the different elements that we have been developing in the two previous chapters.

Assuming **H0'**, Proposition 10.2.17 gives a sequence $(\varepsilon_k)_{k\in\mathbb{N}}$ (occasionally extracted from a preceding sequence of ε) such that, for any $\phi \in C_0^\infty(\mathbb{R}\times\mathbb{R}^d)$,

$$\lim_{k\to\infty} \int_{\mathbb{R}\times\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_k}(t,x)|^2 dxdt \;=\; \sum_{j\in I} \int_{\mathbb{R}\times\mathbb{R}^{2d}} \phi(x)\mu_j(dt,dx,d\xi),$$

where μ_j is a Wigner measure for the concentration of the sequence $(\psi_j^{\varepsilon_k})_{k\in\mathbb{N}}$ whose structure was deeply analysed in Chapter 9.

If **w-H2** holds, then there exist positive measures γ_j on $\times T^*\Lambda_j$ and measurable functions taking values on self-adjoint, positive, trace-class operators

$$\mathfrak{M}_j : \mathbb{R} \times T^*\Lambda_j \ni (t, z, \xi) \longmapsto \mathfrak{M}_j(t, z, \xi) \in \mathcal{L}\left(L^2(N_\xi^*\Lambda_j)\right)$$

satisfying the Heisenberg equation 8.4.6 for initial data $\mathfrak{M}_{0,j}$ such that

$$\mathrm{tr}_{L^2(N_\xi^*\Lambda_j)}\mathfrak{M}_{0,j}(z, \xi) = 1,$$

with $M_{0,j} = \mathfrak{M}_{0,j}\gamma_j$ being the two-microlocal operator-valued measure associated to the concentration of $\psi_{0,j}^{\varepsilon_k}$ over Λ_j. With these measures one can calculate, for any $\phi \in C_0^\infty(\mathbb{R} \times \mathbb{R}^d)$:

$$\int_{\mathbb{R}\times\mathbb{R}^d} \phi(t, x)\mu^j(dt, dx, d\xi) \;=\; \int_{\mathbb{R}\times T^*\Lambda_j} \mathrm{tr}_{L^2\left(N_\xi^*\Lambda_j\right)} \left(m_{\phi_t}(z, \xi)\mathfrak{M}_j(t, z, \xi)\right) \gamma_j(dz, d\xi)dt,$$

with m_{ϕ_t} as defined in Chapter 8. This proves Theorem 8.4.2.

Finally, for Theorem 8.4.3, just switch **w-H2** by **s-H2**, and everything comes from the same reasoning.

Chapter 11

Examples

11.1 Continuities and absolute continuities

Let us start our list of examples of applications of the effective mass theory developed insofar by studying some non-intuitive facts about the Wigner measures and by showing how they can be interpreted in conformity with the general theory of Semiclassical Analysis.

To begin with, we introduced the Wigner measures μ in Chapter 2 as elements in $\mathcal{D}'(\mathbb{R}\times\mathbb{R}^d)$ related to a family of functions $(\Psi^\varepsilon)_{\varepsilon>0}$ in $L^\infty\big(\mathbb{R}, L^2(\mathbb{R}^d)\big)$. Later in Section 2.2, we saw that they are always absolutely continuous with respect to the $\mathbb{R}$ Lebesgue measure in the variable t, which gives $L^\infty\big(\mathbb{R}, \mathcal{D}'(\mathbb{R}^d)\big)$ functions $t \longmapsto \mu_t$, and that sometimes these function may even be continuous. More precisely, in Remark 2.2.1 we explained that, under some conditions on Ψ^ε, this continuity is assured and, further, μ_t results from the concentration of Ψ^ε_t.

Well, Proposition 9.2.4 seems to show that, in our analysis of the Bloch modes, $t \longmapsto \mu_t$ can be taken continuous, since so is $\mathbb{R} \ni t \longmapsto u_{\xi_0,t} \in L^2(\mathbb{R}^d)$. This is not false, but it turns out that, here, μ_t *has nothing to do with the concentration of* u^ε_t, as we will see for $t = 0$.

Example 11.1.1. In the context of Proposition 9.2.4, suppose that $\Lambda = \{\xi_0\}$, where $\xi_0 \neq 0$. Take

$$u^\varepsilon_0 = e^{\frac{i}{\varepsilon}(1+\varepsilon^\alpha)\xi_0\cdot x}\theta(x)$$

with $\theta \in C^\infty_0(\mathbb{R}^d)$, $\|\theta\|_{L^2(\mathbb{R}^d)} = 1$ and $\alpha \in (0,1)$. We have $u_{\xi_0,0} = 0$, which carries that $u_{\xi_0,t} = 0$ for any $t \in \mathbb{R}$ and, consequently, $\mu = 0$, allowing us to choose $\mu_t = 0$ for all t. However, denoting by $\tilde{\mu}$ the Wigner measure associated to the family u^ε_0, we obtain $\tilde{\mu}(x,\xi) = |\theta(x)|^2 dx \otimes \delta(\xi - \xi_0)$.

What would be wrong in our analysis?

The answer is that, unlike in Remark 2.2.1, we did not have any property on u^ε nor on equation (8.3.1) that allowed one to obtain time continuity for the semiclassical limits of u^ε_t (nor even to assure us that they could be taken with the same sequence of ε for every t) and to show that these limits could be used to decompose the previously defined Wigner measure as $\mu = \mu_t\, dt$. What we did was the opposite: first we got an explicit expression for μ, and then we just observed that, among all the possible choices of $t \longmapsto \mu_t$ it admitted (all of them different from one another for up to a zero Lebesgue measure set in $\mathbb{R}$), one happened to be continuous.

Furthermore, this ambiguity within null measure sets implies that, even if we had some link between μ_t and the concentration of the families u^ε_t through some sequence of ε, which we did not, still it would be useless for particular times, as we showed above for $t = 0$, and thus useless for understanding μ_t as an evolution of the semiclassical measure of the initial data u_0^ε, in spite of the fact that these μ_t do evolve according to a well known rule given by our results in Chapter 9.

Example 11.1.2. Keeping the same notations as in Example 11.1.1, take

$$u_0^{\varepsilon,1} = e^{\frac{i}{\varepsilon}\xi_0 \cdot x}\theta(x) \quad \text{and} \quad u_0^{\varepsilon,2} = e^{\frac{i}{\varepsilon}(1+\varepsilon^\alpha)\xi_0 \cdot x}\theta(x).$$

One shows that $\mu^1 \neq \mu^2$, since $\mu^1 \neq 0$, for $u^1_{\xi_0,0} = \theta \neq 0$, and $\mu^2 = 0$, as we have seen. Moreover, we can choose $\mu_t^1(x,\xi) = |u^1_{\xi_0}(t,x)|^2 dx \otimes \delta(\xi - \xi_0)$ and $\mu_t^2 = 0$ for all $t \in \mathbb{R}$, which shows that μ_t^1 and μ_t^2 evolve differently even though $\tilde{\mu}^1 = \tilde{\mu}^2$. Finally, observe that for the first family of data we have $\mu_0^1 = \tilde{\mu}^1$, but, for the second one, $\mu_0^2 \neq \tilde{\mu}^2$, which illustrates that coincidences between $\tilde{\mu}$ and μ_0 are fortuitous unless we have some stronger hypotheses on the concentrating functions that guarantee time continuity for their semiclassical limits along the same sequence of ε.

The persistence of this evolutionary character of the Wigner measure μ and its associates μ_t comes from the fact that the only term that is left in the two-microlocal decomposition of μ is the operator-valued measure M, whose M_t are indeed related to the functions u_t^ε[1] and obtainable through the same sequence of ε for compact times. Yet, the two-microlocal decomposition too is only valid for almost all t, which is clear from the fact that it is obtained under an integral in t and was already stressed in Section 4.6 regarding the measure in sphere ν, so we remain without a perfect link between μ_t and u_t^ε.

In our interpretation, we think of μ_t extracted from μ by imposing continuity on $t \longmapsto \mu_t$ as a "mean" value for the measure to which u_t^ε would concentrate, "averaging" the concentration of $u_{\tilde{t}}^\varepsilon$ over $\tilde{t}$ around t, in smaller and smaller neighbourhoods. This intuition is straightforward when one can take the semiclassical limits of $u_{\tilde{t}}^\varepsilon$ along the same sequence of ε for almost all $\tilde{t}$ near t.

Let us now look closer at the operator-valued measures. As stated in Remark 2.3.3, we know that they induce scalar measures $\mathfrak{m}$ on $\mathbb{R} \times E\Lambda$, which were shown in Lemma 2.3.5 to be always absolutely continuous with respect to the Lebesgue measure on the normal and conormal spaces (and with respect to the time, of course). Here we will see that they may be singular in all other variables by analysing Example 11.1.3 below.

In order to obtain a non-trivial result, it is necessary to suppose $\dim \Lambda > 0$, for, in the case where Λ is just a union of discrete points, it is obvious that $\mathfrak{m}$ cannot be absolutely continuous on the manifold or its cotangent spaces unless it be zero (a fact that, by the way, we used as an argument in Part II to discard the operator-valued measure of the two-microlocal decomposition over the conical singularities).

Example 11.1.3. Assume $\Lambda = \{\xi'' = 0\}$, where $\xi = (\xi', \xi'') \in \mathbb{R}^{d-p} \times \mathbb{R}^p$ with $p > 0$, fix $(x_0', \xi_0') \in \mathbb{R}^{2(d-p)}$ and define

$$u_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{\alpha}{2}(d-p)}}\theta\left(x''\right)\varphi\left(\frac{x' - x_0'}{\varepsilon^\alpha}\right)e^{\frac{i}{\varepsilon}\xi_0' \cdot x'},$$

[1] M_t is the operator-valued measure issued from the concentration of $u^\varepsilon_{\xi_0,t}$, which are unitary transformations of u_t^ε, $u^\varepsilon_{\xi_0,t}(x) = e^{-\frac{it}{\varepsilon^2}\lambda(\xi_0)}e^{-\frac{i}{\varepsilon}\xi_0 \cdot x}u_t^\varepsilon(x)$.

where $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^{d-p})$ and $\theta \in \mathcal{C}_0^\infty(\mathbb{R}^p)$ with $\|\varphi\|_{L^2(\mathbb{R}^{d-p})} = \|\theta\|_{L^2(\mathbb{R}^p)} = 1$. Then, representing $T^*\Lambda$ as the set of points $(x', \xi') \in \mathbb{R}^{2(d-p)}$, the measure M_0 of Theorem 8.3.4 reads:

$$M_0(x', \xi') = |\theta\rangle\langle\theta|\, \delta\left(x' - x_0'\right) \otimes \delta\left(\xi' - \xi_0'\right),$$

or, using the Radon-Nikodym representation $M_0 = \mathfrak{M}_0\gamma$:

$$\gamma(x', \xi') = \delta(x' - x_0') \otimes \delta(\xi' - \xi_0') \quad \text{and} \quad \mathfrak{M}_0(x', \xi') = |\theta\rangle\langle\theta|\,.$$

More generally, we could replace φ and θ so that $\theta = \theta(x', x'')$ in such a manner that $\|\theta(x', \cdot\,)\|_{L^2(\mathbb{R}^p)} = 1$ for any $x' \in \mathbb{R}^{d-p}$ and $\|u_0^\varepsilon\|_{L^2(\mathbb{R}^d)} = 1$, and then we would have $M_0 = \mathfrak{M}_0\gamma$ with:

$$\gamma(x', \xi') = \delta(x' - x_0') \otimes \delta(\xi' - \xi_0') \quad \text{and} \quad \mathfrak{M}_0(x', \xi') = \big|\theta(x', \cdot\,)\big\rangle\big\langle\theta(x', \cdot\,)\big|\,.$$

Finally, since γ is time independent, we will have

$$M_t(x', \xi') = \mathfrak{M}(t, x', \xi')\delta(x' - x_0') \otimes \delta(\xi' - \xi_0')$$

for any t.

Above, the conormal space is $N_{\xi'}^*\Lambda = \mathbb{R}_{x''}^p$, and we will denote by $N_{\xi'}\Lambda = \mathbb{R}_\rho^p$ the normal one. It follows that

$$\mathfrak{m}(t, x, \xi', \rho) = \delta(x' - x_0') \otimes \delta(\xi' - \xi_0') \otimes \tilde{\mathfrak{m}}(t, x'', \rho),$$

giving, for any $a \in S(p)$ and $\Xi \in C_0^\infty(\mathbb{R})$:

$$\begin{aligned} &\operatorname{tr} \left\langle\, M(t, x', \xi')\,,\, \Xi(t)\, a^w\left(x', y, \xi', 0, \partial_y\right) \right\rangle_{\mathbb{R}\times T^*\Lambda} = \\ &\qquad \left\langle\, \delta(\xi'') \otimes \delta(x' - x_0') \otimes \delta(\xi' - \xi_0') \otimes \tilde{\mathfrak{m}}(t, x'', \rho)\,,\, \Xi(t)\, a(x, \xi, \rho) \right\rangle_{\mathbb{R}\times\tilde{E}\Lambda}, \end{aligned}$$

with, naturally, $\tilde{\mathfrak{m}}(t, x'', \rho) = m(t, x'', \rho)dx''d\rho\, dt$ for some appropriate function m (and $\tilde{E}\Lambda$ being basically $E\Lambda$ with an additional fibre $N_{\xi'}\Lambda$ to seize ξ'', that is going to be 0 anyway).

Another interesting feature that we want to explore in Example 11.1.3 is that Theorem 8.3.4 gives:

$$M(t, x', \xi') = \Big|e^{-it\hat{H}(x', \xi')}\theta(x', \cdot\,)\Big\rangle\Big\langle e^{-it\hat{H}(x', \xi')}\theta(x', \cdot\,)\Big|\, \delta(x' - x_0') \otimes \delta(\xi' - \xi_0') \otimes dt,$$

where

$$\hat{H}(x', \xi') = -\frac{1}{2}\nabla_{\xi''}^2\lambda(\xi)\partial_{x''} \cdot \partial_{x''} + V(x)$$

are operators acting on $L^2(N_{\xi'}^*\Lambda) = L^2(\mathbb{R}_{x''}^p)$. In other words, the evolution of the semi-classical measures depends only on the profile θ that the initial data have over the conormal space, the rest constituting a family of coherent states concentrating onto the point (x_0', ξ_0') of $T^*\Lambda$ and thus giving the singular scalar measure γ.

In a final example with coherent states, we go back to the case $\dim \Lambda = 0$ and notice that u_{ξ_0} may be identically equal to zero even if the family $(u_0^\varepsilon)_{\varepsilon>0}$ oscillates along the vector ξ_0:

Example 11.1.4. Define as initial data the family of coherent states centred in (x_0, ξ_0) in the phase space,

$$u_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{d}{4}}}\theta\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right)e^{\frac{i}{\varepsilon}\xi_0 \cdot x},$$

with $\theta \in C_0^\infty(\mathbb{R}^d)$, $\|\theta\|_{L^2(\mathbb{R}^d)} = 1$. Then $u_{\xi_0}(t, \cdot\,) = 0$ for every $\xi_0 \in \mathbb{R}^d$ and Theorem 8.3.1 allows us to conclude that the corresponding densities $|u^\varepsilon|^2$ of solutions to (8.3.1) converge weakly to zero in $L^2_{\text{loc}}(\mathbb{R} \times \mathbb{R}^d)$.

11.2 Hypothesis failure

In this section we shall see what may happen when the assumptions **s-H2** and **w-H2** of Theorems 8.3.1 and 8.3.4 fail, and we will discover that, when the Hessian of λ is allowed to be degenerate, then these results become false. We will focus on the case with $V = 0$ where exact computations may be performed, helping us to depict the mechanisms involved in the process.

11.2.1 The discrete case

Let us suppose that $\dim \Lambda = 0$ and that there is some $\xi_0 \in \Lambda$ for which $\nabla^2\lambda(\xi_0)$ is degenerate, *i.e.*, for which one can find $\omega_0 \in \mathcal{S}^{d-1}$ such that $\nabla^2\lambda(\xi_0)\omega_0 = 0$.

Example 11.2.1. Suppose $\Lambda = \{\xi_0\}$ and let be $\alpha \in [0, 1)$ and $\beta \in \left(\frac{2}{3}, 1\right)$ such that they satisfy $\alpha + \beta < 1$. Choose $\omega_0 \in \ker \nabla^2\lambda(\xi_0)$ with $\|\omega_0\| = 1$ and consider the family of initial data

$$u_0^\varepsilon(x) = \frac{1}{\varepsilon^{\frac{\alpha d}{2}}}\theta\left(\frac{x}{\varepsilon^\alpha}\right)e^{\frac{i}{\varepsilon}(\xi_0+\varepsilon^\beta\omega_0)\cdot x},$$

where $\theta \in C_0^\infty(\mathbb{R}^d)$, $\|\theta\|_{L^2(\mathbb{R}^d)} = 1$. We have $\operatorname{w\,lim}\left(e^{-i\xi_0 \cdot x}u_0^\varepsilon\right) = 0$, so $u_{\xi_0,t} = 0$ for any t and Theorem 8.3.1 would imply $\mu = 0$. However:

- if $\alpha \neq 0$, then
$$\mu(t, x, \xi) = \delta(x) \otimes \delta(\xi - \xi_0) \otimes dt;$$
- if $\alpha = 0$, then
$$\mu(t, x, \xi) = \left|e^{-it\nabla^2\lambda(\xi_0)\partial_x \cdot \partial_x}\theta(x)\right|^2 dx \otimes \delta(\xi - \xi_0) \otimes dt.$$

In both cases, we have provided examples that hypothesis **s-H2** is necessary in the theorem (and in Proposition 9.2.4).

Proof. The proof of these facts relies on the analysis of the product

$$L_t^\varepsilon = \left\langle \operatorname{op}_\varepsilon\left(a\left(x, \xi, \frac{\xi - \xi_0}{\varepsilon}\right)\right)u_t^\varepsilon\, , u_t^\varepsilon\right\rangle,$$

where $a \in S(d)$ and u^ε is a solution to $i\varepsilon^2\partial_t u_t^\varepsilon(x) = \lambda(\varepsilon\partial_x)u_t^\varepsilon(x)$, which is equation (8.3.1) with $V = 0$. Since

$$u_t^\varepsilon(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}e^{-\frac{it}{\varepsilon^2}\lambda(\xi)}u_0^\varepsilon(y)dyd\xi,$$

L_t^ε reads:

$$L_t^\varepsilon = \frac{1}{(2\pi\varepsilon)^{3d}\varepsilon^{d\alpha}} \int_{\mathbb{R}^{7d}} a\left(\frac{x+y}{2}, \xi, \frac{\xi-\xi_0}{\varepsilon}\right) \theta\left(\frac{z}{\varepsilon^\alpha}\right) \overline{\theta\left(\frac{w}{\varepsilon^\alpha}\right)} e^{\frac{it}{\varepsilon^2}(\lambda(\eta)-\lambda(\zeta))} \\ e^{\frac{i}{\varepsilon}\left(\xi\cdot(x-y)+(\xi_0+\varepsilon^\beta\omega_0)\cdot(z-w)+\zeta\cdot(y-z)-\eta\cdot(x-w)\right)} dz\, dw\, d\zeta\, d\eta\, d\xi\, dy\, dx.$$

We perform the variable changes

$$\begin{array}{c} x = \varepsilon^\alpha \tilde{x} \\ y = \varepsilon^\alpha \tilde{y} \\ z = \varepsilon^\alpha \tilde{z} \\ w = \varepsilon^\alpha \tilde{w} \end{array} \quad \text{and} \quad \begin{array}{c} \xi = \xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\tilde{\xi} \\ \zeta = \xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\tilde{\zeta} \\ \eta = \xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\tilde{\eta} \end{array}$$

in order to obtain (dropping the tildes):

$$L_t^\varepsilon = \frac{1}{(2\pi)^{3d}} \int_{\mathbb{R}^{7d}} a\left(\varepsilon^\alpha \frac{x+y}{2}, \xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\xi, \frac{\omega_0 + \varepsilon^{1-\alpha-\beta}\xi}{\varepsilon^{\beta-1}}\right) \theta(z)\, \overline{\theta(w)} \\ e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))} e^{\frac{it}{\varepsilon^2}\Gamma^\varepsilon(\eta,\zeta)} dz\, dw\, d\zeta\, d\eta\, d\xi\, dy\, dx,$$

with

$$\begin{aligned} \Gamma^\varepsilon(\eta,\zeta) &= \lambda\left(\xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\eta\right) - \lambda\left(\xi_0 + \varepsilon^\beta\omega_0 + \varepsilon^{1-\alpha}\zeta\right) \\ &= \varepsilon^{2(1-\alpha)}\left(\nabla^2\lambda(\xi_0)\eta\cdot\eta - \nabla^2\lambda(\xi_0)\zeta\cdot\zeta\right) + \mathcal{O}\left(\varepsilon^{3\beta}\right), \end{aligned}$$

where we have used $\nabla^2\lambda(\xi_0)\omega_0 = 0$ and $\beta < 1-\alpha$. Since $3\beta > 2$, the term in $\mathcal{O}(\varepsilon^{3\beta})$ will be negligible in the phase $e^{\frac{it}{\varepsilon^2}\mathcal{O}(\varepsilon^{3\beta})}$ for compact times.

The situation now depends on whether $\alpha = 0$ or not.

- If $\alpha \neq 0$, making use of a Taylor expansion and by the definition of a, one easily convinces oneself that we have approximatively, for ε small:

  $$L_t^\varepsilon \approx \frac{1}{(2\pi)^{3d}} a_\infty(0,\xi_0,\omega_0) \int_{\mathbb{R}^{7d}} \theta(z)\, \overline{\theta(w)} e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))} \\ e^{\frac{it}{\varepsilon^{2\alpha}}\left(\nabla^2\lambda(\xi_0)\eta\cdot\eta - \nabla^2\lambda(\xi_0)\zeta\cdot\zeta\right)} dz\, dw\, d\zeta\, d\eta\, d\xi\, dy\, dx;$$

  integration in ξ generates a Dirac mass $(2\pi)^d\delta(x-y)$, then integration in y and x generates a Dirac mass $(2\pi)^d\delta(\zeta-\eta)$, integration in η and ζ results in $(2\pi)^d\delta(w-z)$ and a final integration in z gives:

  $$L_t^\varepsilon \approx a_\infty(0,\xi_0,\omega_0)\, \|\theta\|_{L^2(\mathbb{R}^d)},$$

  whence $\mu(t,x,\xi) = \delta(x)\otimes\delta(\xi-\xi_0)\otimes dt$.

- If $\alpha = 0$, similar arguments give, when ε is taken negligible:

  $$L_t^\varepsilon \approx \frac{1}{(2\pi)^{3d}} \int_{\mathbb{R}^{7d}} a_\infty\left(\frac{x+y}{2}, \xi_0, \omega_0\right) e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))} \\ e^{it\left(\nabla^2\lambda(\xi_0)\eta\cdot\eta - \nabla^2\lambda(\xi_0)\zeta\cdot\zeta\right)} \theta(z)\, \overline{\theta(w)} dz\, dw\, d\zeta\, d\eta\, d\xi\, dy\, dx;$$

integration in ξ generates a Dirac mass $(2\pi)^d\delta(x-y)$ and integrations in y, z and w give:

$$L_t^\varepsilon \;\approx\; \frac{1}{(2\pi)^d}\int_{\mathbb{R}^{3d}} a_\infty\left(x,\xi_0,\frac{\omega_0}{\|\omega_0\|}\right) e^{ix\cdot(\zeta-\eta)} e^{it\left(\nabla^2\lambda(\xi_0)\eta\cdot\eta-\nabla^2\lambda(\xi_0)\zeta\cdot\zeta\right)}\hat{\theta}\,(\zeta)\,\overline{\hat{\theta}\,(\eta)} \; d\zeta\, d\eta\, dx;$$

finally, integrating in ζ and η:

$$L_t^\varepsilon \;\approx\; \int_{\mathbb{R}^d} a_\infty\,(x,\xi_0,\omega_0)\left|e^{-it\nabla^2\lambda(\xi_0)\partial_x\cdot\partial_x}\theta(x)\right|^2 dx,$$

implying $\mu(t,x,\xi)=\left|e^{-it\nabla^2\lambda(\xi_0)\partial_x\cdot\partial_x}\theta(x)\right|^2 dx\otimes\delta(\xi-\xi_0)\otimes dt$ as stated.

Of course, in both cases above we took symbols $a\in C_0^\infty(\mathbb{R}^{2d})$ and integrated L_t^ε against $\Xi\in C_0^\infty(\mathbb{R})$ in order to obtain the semiclassical measures. □

It is important to notice that Theorem 8.3.1 becomes rather incomplete than wrong without **s-H2**: one sees from the proof above that μ is given by a two-microlocal decomposition where the only term left is the projection of the measure in sphere:

$$\begin{array}{lll} \nu(t,x,\omega)=\delta\,(\omega-\omega_0)\otimes\delta(x)\otimes dt & \multirow{2}{*}{if} & \alpha\neq 0 \\ \nu(t,x,\omega)=\left|e^{-it\nabla^2\lambda(\xi_0)\partial_x\cdot\partial_x}\theta(x)\right|^2\delta\,(\omega-\omega_0)\otimes dx\otimes dt & & \alpha=0, \end{array}$$

which eventually corroborates the fact that $M=0$, as the theorem affirmed, since $u_{\xi_0,t}=0$ for any t. What is failing here is the dispersivity of the flow in Lemma 9.2.3, which had led us to ignore the contribution of ν to the full Wigner measure, whereas this and the other lemmata in which consisted the proof of Theorem 8.3.1 keep holding.

11.2.2 The continuous case

As usual, we will denote $\xi=(\xi',\xi'')$ with $\xi'\in\mathbb{R}^{d-p}$ and $\xi''\in\mathbb{R}^p$, and suppose that $\Lambda=\left\{\xi\in\mathbb{R}^d:\xi''=0\right\}$, which means that $\nabla\lambda(\xi',0)=0$ for all $\xi'\in\mathbb{R}^{d-p}$. For simplicity, we will take $V=0$ in equation (8.3.1).

Example 11.2.2. Suppose that there is $\xi_0'\in\Lambda$ for which the Hessian of λ is not of full rank, so one can choose $\omega_0\in\mathcal{S}^{p-1}$ such that $\nabla^2_{\xi''}\lambda(\xi_0',0)\omega_0=0$. Consider initial data of the form

$$u_0^\varepsilon(x)=\frac{1}{\varepsilon^{\frac{\alpha p}{2}}}\varphi(x')\,\theta\left(\frac{x''}{\varepsilon^\alpha}\right)e^{\frac{i}{\varepsilon}\left(\xi_0'\cdot x'+\varepsilon^\beta\omega_0\cdot x''\right)},$$

where $\alpha\in[0,1)$ and $\beta\in\left(\frac{2}{3},1\right)$ are such that $\alpha+\beta<1$, and $\theta\in C_0^\infty(\mathbb{R}^p)$, $\varphi\in C_0^\infty(\mathbb{R}^{d-p})$, with $\|\theta\|_{L^2(\mathbb{R}^p)}=\|\varphi\|_{L^2(\mathbb{R}^{d-p})}=1$. In this case we have:

- if $\alpha\neq 0$, then

$$\mu(t,x,\xi)=\left|\varphi\left(x'\right)\right|^2 dx'\otimes\delta(x'')\otimes\delta(\xi'-\xi_0')\otimes\delta(\xi'')\otimes dt;$$

- if $\alpha=0$, then

$$\mu(t,x,\xi)=\left|\varphi(x')\,e^{-it\nabla^2_{\xi''}\lambda(\xi_0',0)\partial_{x''}\cdot\partial_{x''}}\theta\left(x''\right)\right|^2 dx\otimes\delta(\xi'-\xi_0')\otimes\delta(\xi'')\otimes dt;$$

whilst in both cases one has $M_0 = 0$, so Theorem 8.3.4 would give $\mu = 0$, a contradiction.

Proof. Again, denoting u^ε the solution to $i\varepsilon^2\partial_t u_t^\varepsilon(x) = \lambda(\varepsilon\partial_x)u_t^\varepsilon(x)$ with initial data u_0^ε, the proof relies on the analysis of the integral

$$L_t^\varepsilon = \left\langle \mathrm{op}_\varepsilon\left(a\left(x,\xi,\frac{\xi''}{\varepsilon}\right)\right)u_t^\varepsilon\,,u_t^\varepsilon\right\rangle,$$

which reads

$$\begin{aligned} L_t^\varepsilon \;=\; & \frac{1}{(2\pi\varepsilon)^{3d}\varepsilon^{p\alpha}}\int_{\mathbb{R}^{7d}} a\left(\frac{x+y}{2},\xi,\frac{\xi''}{\varepsilon}\right)e^{\frac{it}{\varepsilon^2}(\lambda(\eta)-\lambda(\zeta))}\varphi(z')\overline{\varphi(w')}\,\theta\left(\frac{z''}{\varepsilon^\alpha}\right)\overline{\theta\left(\frac{w''}{\varepsilon^\alpha}\right)} \\ & e^{\frac{i}{\varepsilon}\left(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w)+\xi_0'\cdot(z'-w')+\varepsilon^\beta\omega_0\cdot(z''-w'')\right)}dz\,dw\,d\zeta\,d\eta\,d\xi\,dy\,dx, \end{aligned}$$

We perform the change of variables

$$\begin{array}{rcl} x''=\varepsilon^\alpha\tilde{x}'' & & \xi''=\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\tilde{\xi}'' & & \xi'=\xi_0'+\varepsilon\tilde{\xi}' \\ y''=\varepsilon^\alpha\tilde{y}'' & \text{and} & \zeta''=\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\tilde{\zeta}'' & \text{and} & \zeta'=\xi_0'+\varepsilon\tilde{\zeta}' \\ z''=\varepsilon^\alpha\tilde{z}'' & & \eta''=\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\tilde{\eta}'' & & \eta'=\xi_0'+\varepsilon\tilde{\eta}' \\ w''=\varepsilon^\alpha\tilde{w}'' & & & & \end{array}$$

and obtain (letting the tildas down):

$$\begin{aligned} L_t^\varepsilon \;=\; & \frac{1}{(2\pi)^{3d}}\int_{\mathbb{R}^{7d}} a\left(\frac{x'+y'}{2},\varepsilon^\alpha\frac{x''+y''}{2},\xi_0'+\varepsilon\xi',\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\xi'',\frac{\omega_0+\varepsilon^{1-\alpha-\beta}\xi''}{\varepsilon^{1-\beta}}\right) \\ & e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))}e^{\frac{it}{\varepsilon^2}\Gamma^\varepsilon(\eta,\zeta)}\varphi(z')\overline{\varphi(w')}\,\theta\left(z''\right)\overline{\theta\left(w''\right)}dz\,dw\,d\zeta\,d\eta\,d\xi\,dy\,dx, \end{aligned}$$

where, using the assumptions on ξ_0' and ω_0,

$$\begin{aligned} \Gamma^\varepsilon(\eta,\zeta) &= \lambda(\xi_0'+\varepsilon\eta',\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\eta'')-\lambda(\xi_0'+\varepsilon\zeta',\varepsilon^\beta\omega_0+\varepsilon^{1-\alpha}\zeta'') \\ &= \varepsilon^{2(1-\alpha)}\left(\nabla^2_{\xi''}\lambda(\xi_0',0)\eta''\cdot\eta''-\nabla^2_{\xi''}\lambda(\xi_0',0)\zeta''\cdot\zeta''\right)+\mathcal{O}(\varepsilon^{3\beta}), \end{aligned}$$

the term $\mathcal{O}(\varepsilon^{3\beta})$ generating a negligible phase in $e^{\frac{it}{\varepsilon^2}\mathcal{O}(\varepsilon^{3\beta})}$ for compact times, as $\beta > \frac{2}{3}$.

Again, the analysis continues differently depending on α being 0 or not.

- If $\alpha \neq 0$, one shows that, when ε is small:

$$\begin{aligned} L_t^\varepsilon \;\approx\; & \frac{1}{(2\pi)^{3d}}\int_{\mathbb{R}^{7d}} a_\infty\left(\frac{x'+y'}{2},0,\xi_0',0,\omega_0\right)e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))}\varphi(z')\overline{\varphi(w')} \\ & e^{\frac{it}{\varepsilon^{2\alpha}}\left(\nabla^2_{\xi''}\lambda(\xi_0',0)\eta''\cdot\eta''-\nabla^2_{\xi''}\lambda(\xi_0',0)\zeta''\cdot\zeta''\right)}\theta\left(z''\right)\overline{\theta\left(w''\right)}dz\,dw\,d\zeta\,d\eta\,d\xi\,dy\,dx. \end{aligned}$$

Integration in ξ generates a Dirac mass $(2\pi)^d\delta(x-y)$, then integrations in y and x'' generate a Dirac mass $(2\pi)^p\delta(\zeta''-\eta'')$ and we obtain, integrating in η'',

$$\begin{aligned} L_t^\varepsilon \;\approx\; & \frac{1}{(2\pi)^{2d-p}}\int_{\mathbb{R}^{5d-2p}} a_\infty\left(x',0,\xi_0',0,\omega_0\right)e^{i(\zeta'\cdot(x'-z')-\eta'\cdot(x'-w')-\zeta''\cdot(z''-w''))} \\ & \varphi(z')\overline{\varphi(w')}\,\theta\left(z''\right)\overline{\theta\left(w''\right)}dz\,dw\,d\zeta\,d\eta'\,dx', \end{aligned}$$

and proceeding like that for all the other variables:

$$L_t^\varepsilon \;\approx\; \int_{\mathbb{R}^{d-p}} a_\infty\left(x',0,\xi_0',0,\omega_0\right)|\varphi(x')|^2dx'.$$

- If $\alpha = 0$, similarly we have:

$$L_t^\varepsilon \approx \frac{1}{(2\pi)^{3d}} \int_{\mathbb{R}^{7d}} a_\infty \left(\frac{x+y}{2}, \xi_0', 0, \omega_0\right) e^{i(\xi\cdot(x-y)+\zeta\cdot(y-z)-\eta\cdot(x-w))} \varphi(z')\overline{\varphi(w')}$$
$$e^{it\left(\nabla^2_{\xi''}\lambda(\xi_0',0)\eta''\cdot\eta''-\nabla^2_{\xi''}\lambda(\xi_0',0)\zeta''\cdot\zeta''\right)} \theta\left(z''\right)\overline{\theta\left(w''\right)} dz\, dw\, d\zeta\, d\eta\, d\xi\, dy\, dx.$$

Integration in ξ generates a Dirac mass $(2\pi)^d\delta(x-y)$, whence

$$L^\varepsilon \approx \frac{1}{(2\pi)^{2d}} \int_{\mathbb{R}^{5d}} a_\infty \left(x, \xi_0', 0, \omega_0\right) e^{i(\zeta\cdot(x-z)-\eta\cdot(x-w))} \varphi(z')\overline{\varphi(w')}$$
$$e^{it\left(\nabla^2_{\xi''}\lambda(\xi_0',0)\eta''\cdot\eta''-\nabla^2_{\xi''}\lambda(\xi_0',0)\zeta''\cdot\zeta''\right)} \theta\left(z''\right)\overline{\theta\left(w''\right)} dz\, dw\, d\zeta\, d\eta\, dx,$$

from where one recognizes that

$$L_t^\varepsilon \approx \int_{\mathbb{R}^d} a_\infty\left(x, \xi_0', 0, \omega_0\right) \left|\varphi(x')\, e^{-it\nabla^2_{\xi''}\lambda(\xi_0',0)\partial_{x''}\cdot\partial_{x''}} \theta\left(x''\right)\right|^2 dx.$$

The last step to obtain the Wigner measures is to restrict the calculations to $a \in C_0^\infty(\mathbb{R}^{2d})$ and integrate L_t^ε in time against some $\Xi \in C_0^\infty(\mathbb{R})$.

In order to show that $M_0 = 0$, it suffices to observe that, either for $\alpha \neq 0$ or $\alpha = 0$, L_0^ε comprehends only the term of the measure on sphere, and not the operator-valued one. □

In the spirit of the comments made in the end of the previous section for the discrete case, here too one notices that Theorem 8.3.4 is rather incomplete than merely invalid without **w-H2**. In this case, the microlocal measures in sphere are:

$$\begin{array}{ll} \nu(t,x,\xi',\omega) = |\varphi(x')|^2 dx' \otimes \delta(x'') \otimes \delta(\xi'-\xi_0') \otimes \delta\left(\omega-\omega_0\right) \otimes dt & \alpha \neq 0 \\ \nu(t,x,\xi',\omega) = \left|\varphi(x')\, e^{-it\nabla^2_{\xi''}\lambda(\xi_0',0)\partial_{x''}\cdot\partial_{x''}}\theta\left(x''\right)\right|^2 dx \otimes \delta(\xi'-\xi_0') \otimes \delta\left(\omega-\omega_0\right) \otimes dt\ , & \alpha = 0. \end{array}$$

What fails now is the same dispersivity of the flow in Lemma 9.4.6, more explicitly in Proposition 9.4.7; all the other accessory results in which consisted the proof of the theorem keep holding.

In this sense, we can still think of Theorems 8.3.1 and 8.3.4 as genuine, though partial results, *i.e.*, we do have part of the energy of the concentrated u^ε obeying to effective mass equations, but also other terms of a more difficult description. Remark, finally, that both in the discrete and in the continuous cases we could find situations, namely $\alpha \neq 0$, where the measures were singular with respect to the conormal variable x or x'', respectively. As we discussed in Example 11.1.3, singularity in these variables is forbidden by Lemma 2.3.5, so we could in these cases at least identify parts of the full measure that *are not* due to the operator-valued measures submitted to the effective mass equations.

Conclusion and Perspectives

In the first part of this thesis we completed the dynamical study – previously undertook in [45] – of Wigner measure propagation for solutions of the Schrödinger equation with conical potentials, and showed in Theorems 3.2.1 and 3.2.4 that these measures are transported by two different Hamiltonian flows, one over the bundle cotangent to the singular set and the other elsewhere in the phase space, up to a transference phenomenon between these two regimes that may arise whenever trajectories in the outsider flow lead in or out the bundle.

We exhausted the question concerning the trajectory splitting by giving a complete scheme for classifying the possible flow behaviours at the singularities, based on Theorems 3.3.3 and 3.3.4, and by furnishing in Theorem 3.4.1 examples where semiclassical measures linked to particular families of initial data take distinct paths after a common trajectory they were following splits.

There remains, however, a point to be enlightened, which is to know whether and under which conditions it is possible for a measure being propagated by the exterior flow to be retained over the singular cotangent bundle or conversely. This problem was partially solved with Theorem 3.3.2, where we saw that in some cases the measures are not allowed to stay on the singularities, illustrated in Example 5.3.5. We also have cases, like in Examples 5.3.1 and 5.3.3, where a measure initially over the singularity is not allowed to leave it due to the restrictive nature of the Hamiltonian flow it is submitted to.

Yet some situations, like those in Examples 5.3.2 and 5.3.4, cannot be treated neither with the theorem nor with the classical flow's constraints. It is thus convenient for a subsequent work either to seek examples where the Wigner measures swap from one regime to the other, or to prove that it is not possible – which we consider to be more likely, seeing the dispersive character of both the Schrödinger equation in general and the Hamiltonian flow in any neighbourhood of the cotangent bundle in these cases, which makes the situation of staying over the singularity "too unstable" to be durable.

Besides, in the process of describing in detail the Wigner measures over the singularities, we interpreted the two-microlocal measure in sphere ν as a density around the analysed set, as if it gave the directions from which the mass is concentrating onto it. Insofar, this interpretation is purely formal, since there has been no concrete results grounding quantitatively the link between these directions and the distribution of ν around the singular manifold's normal bundle in sphere; not that we know, at least. In [31] we will aim to address this matter in a clearer way.

In the second part, we presented a work in collaboration with Dr. Clotilde Fermanian and Dr. Fabricio Macià where we analysed a Schrödinger-like equation pertinent to the semiclassical study of the dynamics of an electron in a crystal with impurities. It was shown that in the limit where the characteristic length of the crystal's lattice can be considered sufficiently small with respect to the variation of the exterior potential modelling the impurities, then this equation is approximated by an effective mass equation, or, more generally, that its solution decomposes in terms of Bloch modes, each of them satisfying an effective mass equation specifically assigned to its Bloch energy.

In order of increasing complexity, Theorem 8.3.1 contains the result for an electron in a band with only one isolated Bloch energy level with isolated critical points; in Theorem 8.3.4 we are still in a band with one single level, but now the critical points form a manifold with strictly positive dimension. Theorem 8.4.2 is a generalization of this fact for an isolated band with many (possibly infinitely many) isolated energy levels. As before, if the energy levels' critical points are isolated, then one can state this result in a simpler way, as in Theorem 8.4.3.

A more general result extending these theorems for isolated bands that allow their energy levels to cross is postponed to a future publication.

Further, of independent interest is the fact that our results can quantify the lack of regularization of high frequency features under critical points that affect the solutions' concentration. Smoothing effects usually come along with dispersive equations, but as we saw in Remark 8.3.3, they fail over points where a flow through which the Wigner measures are invariant is non-dispersive. In Chapter 11 we illustrated the applications of our results with concrete examples and showed how the existence of points over which the Hessian of the Bloch energy is not of full rank allows part of the concentrated mass not to obey to the effective mass equations.

Finally, we would like to point out that writing this thesis was intensively satisfying from an intellectual point of view, in the sense that it provided us with a genuine understanding of Classical Mechanics as one of many possible clear and rigorously defined limits of Quantum Mechanics. Far more than justifying the classical theory, whose attested accuracy in so broad situations allows it to stand up by itself and must be emphasised, it gave us new insights into the way we should look at Quantum Mechanics, a machinery behind a macroscopic, yet intrinsically statistical description of nature.

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