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WIDTHS OF SEMICLASSICAL EXCITED RESONANCES

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Introduction

What are resonances

This work is devoted to the study of quantum resonances, from different points of view, of the semiclassical Schrödinger operator

$$P := -h^2\Delta + V(x)$$

in one and several dimensions.

In a quantum model, a molecule is described by a wave function $\psi(t, x, y)$ that solves the time-dependent Schrödinger Equation,

$$\begin{cases} ih\partial_t\psi = H\psi \\ \psi|_{t=0} = \psi_0 \end{cases}, \tag{0.0.1}$$

where $x \in \mathbb{R}^{3n}, y \in \mathbb{R}^{3p}$ represent the positions of, respectively, the nuclei and the electrons; this state function satisfies the normalization condition $||\psi_t(\cdot)||_{L^2} = 1$ and on every open set $\Omega \in \mathbb{R}^{3n} \times \mathbb{R}^{3p}$ its integral is the probability of presence in Ω. With some assumptions the total energy of the system is represented by a quantum Hamiltonian

$$H = -\sum_{j=1}^{n} \frac{h^2}{2M_j}\Delta_{x_j} - \frac{h^2}{2m}\sum_{k=1}^{p}\Delta_{y_k} + W(x, y), \tag{0.0.2}$$

that contains the interactions between the particles in the molecule and eventually external fields, is self-adjoint in L^2, and the solution $\psi_t = e^{-itH/h}\psi_0$ depends on the choice of the initial state ψ_0.

For the **Stationary states** the probability is "stationary", the wave packet remains localized for all time $t \in \mathbb{R}$: $|\psi(x, y)|^2 = |\psi_0(x, y)e^{-itH/h}|^2 = |\psi_0(x, y)|^2$; ψ_0 is an eigenfunction of H, $H\psi_0 = E\psi_0$ with E real, and the probability remains the same. If the particle does not remain localized in a small region of space, but diffuses through the entire system, we are in presence of **Scattering states**; in this case $\psi_0 \in \bigcap_{E\in\mathbb{R}} (\ker(H - E))^{\perp}$, and it can be shown that, for any compact set $K \in$

$\mathbb{R}^{3n} \times \mathbb{R}^{3p}$,

$$\| \psi_t \|^2_{L^2(K)} \longrightarrow 0 \quad \text{as} \quad |t| \longrightarrow +\infty. \tag{0.0.3}$$

A **Metastable state** ψ_1 is a solution to the Schrödinger equation which corresponds to a complex number $\rho, Im\rho < 0$; more specifically there are states ψ_1 with some particular behavior at infinity, such that $\psi_1 \notin L^2$ are solutions of $H\psi_1 = \rho\psi_1$. If we set $\rho = E - ib$, the time evolution should be written $\psi(t) = e^{(-it(E-ib))/\hbar}\psi_0$, so that the probability of presence at time t will be

$$\frac{|\psi(x,y)|^2}{|\psi_0(x,y)|^2} = e^{-bt/h} \underbrace{\longrightarrow}_{t\to\infty} 0. \tag{0.0.4}$$

Thus the quantity $\frac{h}{b}$ gives us an idea of the life time of the molecule, where $b = \text{Im } \rho$ is the width, which is important to estimate.

In Physics the notion of quantum resonance comes namely from the behaviour of quantities related to some scattering experiments (total scattering cross sections); at certain energies these quantities present peaks, which are described by a Lorentzian shaped function of the type

$$\lambda \mapsto \frac{1}{(\lambda - Re\rho)^2 + (Im\rho)^2} = \frac{1}{|\lambda - \rho|^2}, \tag{0.0.5}$$

where the imaginary part of ρ gives the inverse of the amplitude of such peaks. From the physical point of view resonances are also associated to metastable states, i.e. states that slowly decay, and their life-time is given by the inverse of the absolute value of the imaginary part (width) of the resonance. A typical resonance situation occurs when a quantum particle with energy E is trapped within a potential well with finite barrier of a given size; this is described by a quantum state ψ_t with initial condition ψ_0 localized in the potential well $W(E)$, such that ψ_t remains in W for a very long time and will then decay away from W thanks to the tunneling effect.

Resonances appear in almost all areas of quantum physics: the theory of atoms and molecules, nuclear and elementary particle physics, with applications from the theory of solids up to quasinormal modes of black holes. These complex values for energies appeared in relatively old works (for instance in [Ga], to explain the energy decay of an unstable atomic nucleus by α-particle emission), but in the $1970'$ and the $1980'$ was the most intense research period where the resonances were rigorously understood as a basic concept of modern physics; Aguilar and Combes [AgCo] and Balslev and Combes [BaCo] gave a rigorous notion of resonances: they used dilation analytic technique to prove the absence of singular continuous spectra for 2- and

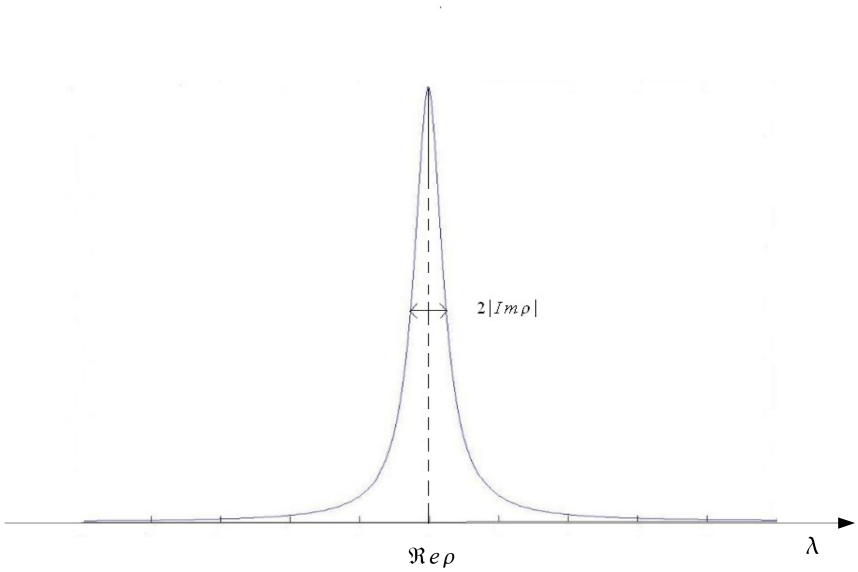


Figure 1: Breit-Wigner peak

N-body Schrödinger operators. The Coulomb potential centered at the origin is dilation analytic, therefore this theory worked well for atoms. In [Sim], Simon applied these methods to define quantum resonances, and one of the first application was to the helium atom and other multielectron atoms. Through the contribution of various researcher the spectral deformation theory, which was first formulated for the dilation group, could be applied to distortion analytic potentials. Hunziker in [Hu] gave a significant contribution to relax and extend the previous formulations, by analysing those different techniques in order to construct the meromorphic extension of the matrix elements of the resolvent of P, and since then various notions of resonances were introduced and their mathematical theory in the generalized semiclassical regime has been applied to many problem, with different approaches. Among the problems of 2-body systems, resonances in the Stark effect, Zeeman effect and magnetic fields were studied in [GrGr], [Si], [HeSj2]; resonances in the Born-Oppenheimer approximation for molecules were studied by Martinez in [Ma3], [Ma4], and in a model of molecular dissociation by Klein ([Kl]).

Through the Born-Oppenheimer approximation ([BoOp]), the spectral properties of the molecular Hamiltonian can be reduced to the study of smooth pseudodifferential operators (e.g. in [KMSW]). Roughly speaking, it consists in reducing the problem of the behaviour of such systems, by "sending" the mass of the heavy particles to $+\infty$. Thus we are led to the study of a cut out Hamiltonian as in (0.0.2), where the last two terms represent the electronic Hamiltonian

$$Q(x) = -\Delta_y + W(x, y), \tag{0.0.6}$$

and the study of $P(h) = H$ can be approximately reduced, when h is small enough, to the one of the family of operators $-h^2\Delta_x + \lambda_j(x), j = 1, ..., N$, where $\lambda_1(x) < \lambda_2(x) \leq ... \leq \lambda_N(x)$ are the (so called electronic levels) first N discrete eigenvalues of $Q(x)$. We are interested in the spectral properties of $P(h)$ near a fixed energy level E. (This method allows us to deal only with $\lambda_j(x)$ verifying $\inf_{x\in R^n} \lambda_j(x) \leq E$). The minimums of λ_j can be physically interpreted as the equilibrum positions of the nuclei around which those will gravitate in a molecular system. Then the spectral study of $P(h)$ can be reduced to that of semiclassical analytic pseudodifferential matrix operator $F(z)$, and its principal part equals the diagonal matrix (up to a $O(h^2)$) $\mathrm{diag}(-h^2\Delta_x + \lambda_j(x))_{1\leq j\leq N}$ corresponding to the original intuition of Born and Oppenheimer. Then we have the following equivalence:

$$z \in \sigma(P(h)) \Longleftrightarrow z \in \sigma(F(z)). \tag{0.0.7}$$

The way in which the spectral reduction of $P(h)$ and this equivalence are obtained

relies on the construction of a matrix operator, the so-called Grushin operator, acting on a greater space by means of the eigenfunctions of $Q(x)$ associated with the eigenvalues $\lambda_1(x), \lambda_2(x), ..., \lambda_N(x)$.
This is the Feshbach method which is also used in several situations to study the eigenvalues and resonances of $P(h)$ in the semiclassical limit where the potential function $W(x, y)$ can be of different types. WKB type expansions for the eigenvalues and resonances of $P(h)$ are obtained by virtue of the Feshbach method and the pseudodifferential operator calculus.

From the mathematical point of view the question concerning Born-Oppenheimer approximation studied in [Ma3] and [Ma4], was inspired by the microlocal treatment of semiclassical spectral problems in [HeSj1]; a first attempt to justify rigorously the Born-Oppenheimer approximation was made in [CDS] for the diatomic molecule. Later again the same microlocal method gave rise to a complete adaption to the case of Coulomb interactions in [KMSW]. It was also natural to compare the different notions of resonances (which in fact coincide, see [HeMa] for the proof): poles of the meromorphic extension from the upper complex half-plane of the matrix element of the resolvent $(P - z)^{-1}$ as in [Hu], or points z of the complex plane, for which $(P(h) - z)$ is not bijective under certain assumption for the hamiltonian, defined as a Fredholm operator on modified Sobolev spaces; this last definition appeared in [HeSj2] and allowed the autors to apply the semiclassical microlocal calculus to typical problems associated to resonances, for instance the so-called "Shape Resonances", the subject of our first chapter: a scalar Hamiltonian ($N = 1$, one electric level) admits the previous situation; the potential presents the geometric shape of a *Well in an Island.* The resonant state describes a quantum particle, concentrated in a potential well for a long period, but then escaping to the sea (classically allowed region outside the island) by tunneling effect. This effect is reflected by the width of the resonance.
The study of shape resonances is a rather old subject in semiclassical analysis, and since the years 80's many mathematical works have been done in order to both locate them and estimate their widths (see, e.g., [AsHa, CDKS, HeSj2, HiSi, FLM] and references therein). In particular, one should mention the work [CDKS], where the existence of shape resonances exponentially close to the real axis is proved, and the work [HeSj2], where a more refined analysis leads to optimal estimates on the widths of resonances that are near a local minimum of the potential. For more excited shape resonances, however, only lower bounds on their widths are available

in general, except for the one-dimensional case where the exact asymptotic behavior can be determined : see [Se].

The purpose of the first chapter is to extend some of the results of [Se] to the multidimensional case. More precisely, considering the semiclassical Schrödinger operator $P := -h^2\Delta + V(x)$ on $L^2(\mathbb{R}^n)$ with $n \geq 1$, we plan to produce optimal exponential estimates on the widths of highly excited shape resonances, that is, shape resonances that tend to an energy E_0 greater than the local minimum of the potential V. In contrast with [Se], here we assume that the potential well (that is, the bounded component U of $\{V \leq E_0\}$) is connected, excluding the situation of possible interacting wells. In this situation, the general multidimensional result says that any resonance $\rho = \rho(h)$ that tends to E_0 as $h \to 0_+$ is such that, for any $\varepsilon > 0$, one has,

$$|\text{Im } \rho| \leq \mathcal{O}(e^{-(2S_0-\varepsilon)/h})$$

uniformly as $h \to 0_+$. Here, $S_0 > 0$ is the Agmon distance (that is, the degenerate distance associated with the pseudo-metric $\max(V - E_0, 0)dx^2$) between U and the unbounded component $\mathcal{M}$ of $\{V \leq E_0\}$.

In other words ρ satisfies,

$$\limsup_{h\to 0_+} h \ln |\text{Im } \rho| \leq -2S_0. \tag{0.0.8}$$

When $n = 1$, this result is improved into (see [Se], Theorem 0.2),

$$\lim_{h\to 0_+} h \ln |\text{Im } \rho| = -2S_0. \tag{0.0.9}$$

Here we plan to extend this improvement to the multidimensional case. Because of (0.0.8), all we need to prove is that, for any $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$ such that,

$$|\text{Im } \rho| \geq \frac{1}{C_\varepsilon} e^{-(2S_0+\varepsilon)/h}, \tag{0.0.10}$$

for all $h > 0$ small enough.

In order to produce such a good lower bound, when $n \geq 2$ it is necessary to add an assumption on the size of the resonant state inside U. This assumption is actually implied by a geometric condition on the classical Hamilton flow above U (see Remark 2.3.3) that is automatically satisfied in the one-dimensional case. Roughly speaking, this condition says that the energy shell $\Sigma_{E_0} := \{(x, \xi) \in \mathbb{R}^{2n}\,;\, \xi^2 + V(x) = E_0\}$ is sufficiently well covered by the classical Hamilton flow, in the sense that any open set intersecting Σ_{E_0} is flowed over a whole neighborhood of Σ_{E_0} (this can be understood as a kind of ergodicity of the flow on Σ_{E_0}).

From a technical point of view, this problem is very close to that of estimating the tunneling for a symmetric double-wells at high excited energies, as considered e.g. in [Ma1] (and indeed, part of our argument will use the results of [Ma1]). However, an additional difficulty comes from the fact that here, the quantity we have to study mainly involves the size of the resonant state in $\mathcal{M}$.

In the semiclassical regime, almost all the tunneling occurs along a small neighborhood of the geodesic curves from the well to the set of points of the boundary of the island where the Agmon distance from the well reaches its minimum. Since Im ρ can be represented in terms of the corresponding resonant state as in formula (10.65) in [HeSj2] (see 2.4.5), where it is shown that the solution coming from the well can be evaluated and compared to the resonant state with a good approximation, one can use the microlocal calculus to propagate the estimate to the well.
Our work will essentially consist in evaluating the size of the resonant state in $\mathcal{M}$ as $h \to 0$ and propagating this evaluation up to that in U, through the barrier $\mathcal{B} := \{V > E_0\}$. The results of [Ma1] permits us to connect the size of the state in $\mathcal{B}$ to that in U only, but not its size in $\mathcal{M}$ to that in $\mathcal{B}$. Indeed, it appears that the argument of [Ma1] (which is typically an argument of propagation of microlocal analyticity) does not seem easy to adapt for this last step. However, following an idea already present in [DGM], one can develop some explicit Carleman-type inequalities that permits us to cross the border between $\mathcal{M}$ and $\mathcal{B}$, and to conclude.
Resonances in quantum mechanical systems are often related to bounded orbits in a corresponding classical system. This idea has been applied to various geometrical situations. Resonances for the Laplace-Beltrami operator on $\mathbb{R}^n$ with certain spherically symmetric Riemannian metrics, such that there exists families of trapped geodesics, were studied by De Bièvre and Hislop ([DeBH]); resonances generated by the maximum point of the potential usually called "Barrier-Top" resonances have been studied at first by Briet, Combes, and Duclos [BCD2] and Sjöstrand [Sj2]. This is a case of resonances generated by closed, hyperbolic trajectories, which were analyzed by [GSj].
The second chapter is devoted to the study of a different geometrical situation, more similar to the barrier-top resonances problem, involving a singularity. It turns out that the imaginary part of the resonances is much larger than that of those created by a regular barrier-top. The underlying idea comes from the studies of [Kl], [GrMa], [FMW] on the theory of the molecular predissociation, where two potential intersect transversally. Moreover, in the main result of this chapter we follow the computations of [FMW] very closely, in order to give the proof of the theorem 3.4.1.

First of all we consider a linear wedge barrier, a geometrical form of the potential with a singularity at the origin ($V(x) = -|x|$). The construction of the solutions of Schrödinger equation is based on expressions that involve the Airy functions Ai, solutions of the second order differential equation

$$\frac{d^2u}{dx^2} = xu. \tag{0.0.11}$$

By computing the connection formulas at the singular point, it turns out that the transmission coefficient is given in terms of an explicit expression, involving Airy functions and their derivatives. The zeros of both these functions, that are real and negative, lead to singularities of the resolvent kernel, thus give rise to resonances for the Schrödinger operator. They will be localized on a rotated line with an angle of $-\frac{2\pi}{3}$, and one can notice an analogy with the energy levels associated to a specular linear potential well $V = |x|$. We assume then a more general linear geometrical form for the potential barrier, acting at first a unilateral dilation, then a complete unsymmetric generalization:

$$V(x) := \begin{cases} -\alpha_2 x & x \geq 0, \\ \alpha_1 x & x < 0 \quad (\alpha_1, \alpha_2) > 0. \end{cases} \tag{0.0.12}$$

In these cases resonances turn out to be zeros of a much more complicated expression, that can't be directly connected with zeros of Ai, Ai'. The next step consists in generalizing the previous constructions and improve the computation, in order to refine the theorem (3.2.11) in a more general case.
Using a method due to Yafaev [Y] (see also [FMW]), and based on a special change of variable, we construct an outgoing solution on $(-\infty, 0]$, and another one on $[0, \infty)$. Then, the quantization condition simply consists in writing that their Wronskian at 0 vanishes. Since these functions are constructed in an iterative way, and their first approximations are given by Airy functions, we obtain a corresponding approximation of the resonances. For the generalization we consider the potential $V = V_1$ in $x < 0, V = V_2$ in $x \geq 0$, where

- V_j are analytic in regions Γ_j,

  $$\Gamma_{1,2} := \{x \in \mathbb{C}; |\mathrm{Im}\, x| < \delta_0 \langle \mathrm{Re}\, x \rangle\} \cap [\pm \mathrm{Re}\, x > -\delta_1], \tag{0.0.13}$$

  for some $\delta_j > 0$;

- there are constants $V_1^-, V_2^+ < 0$:

  $$V_1(x) \to V_1^- \qquad (\mathrm{Re}\, x \to -\infty \quad \text{in} \quad \Gamma_1); \tag{0.0.14}$$

  $$V_2(x) \to V_2^+ \qquad (\mathrm{Re}\, x \to \infty \quad \text{in} \quad \Gamma_2), \tag{0.0.15}$$

and V is a real valued continuous function on the real line satisfying

$$V(x) < 0 \quad (x \in \mathbb{R} \setminus 0), \qquad V(0) = 0, \tag{0.0.16}$$

with linearization $V_0(x) = V(x; \alpha_1, \alpha_2)$ at $x = 0$, i.e.:

$$V_0(x) = \alpha_1 x \quad (x < 0), V_0(x) = -\alpha_2 x \quad (x > 0), \tag{0.0.17}$$

for some $\alpha_j > 0 \quad (j = 1, 2)$. Thus our final result is theorem (3.4.1):

$$\text{Set} \quad D_h(C_0) = \left[-C_0 h^{2/3}, C_0 h^{2/3}\right] - i\left[0, C_0 h^{2/3}\right]; \tag{0.0.18}$$

Then for any $C_0 > 0$, h sufficiently small, the operator $P = -h^2\partial_x^2 + V(x)$ has resonances

$$Res(P) \cap D_h(C_0) = \{\lambda_k(h); k \in \mathbb{N}\} \cap D_h(C_0), \tag{0.0.19}$$

$$\text{where} \quad \lambda_k(h) \sim h^{\frac{2}{3}} \sum_n c_{k,n} h^{\frac{n}{3}}. \tag{0.0.20}$$

The leading term $\lambda_{k,0}(h) = h^{2/3}c_{k,0}$ coincides with the resonances for the linearized operator $P_0 = -h^2\partial_x^2 + V_o$.

In leading order, this reduces in fact to the explicitly solvable linear wedge problem. By developing a different WKB construction we will be able to extend this result to potentials $V(x) \sim \alpha_\pm x$. We expect that this type of results appears in the Born-Oppenheimer approximation, by constructing resonances λ_k for a two-level problem with a crossing (described by a matrix case) in a window where $\operatorname{Im} \lambda_k \in [-Ch^{\frac{2}{3}}, 0]$, in analogy with the theory discussed in [FMW].

Chapter 1

Background of Resonances

1.1 Analytic Distorsion

One of the useful tool to study the theory of resonances for the Schrödinger operator $P(h) = -h^2\Delta + V$ on $L^2(\mathbb{R}^n)$ is the spectral deformation, developed thanks to the "analytic dilation" technique ([AgCo], [BaCo]) and later with the more general "analytic distorsion" ([Hu]); it allows us to identify resonances of a selfadjoint operator $\mathbf{P}$ with complex eigenvalues of a closed operator $\mathbf{P}_\theta$, obtained by spectral deformation, and these eigenvalues are related to the poles of the meromorphic continuation of the matrix elements of the resolvent.

The basic idea is to consider one-parameter families of diffeomorphisms on $\mathbb{R}^n$, that admit an extension on a neighborhood of $\mathbb{R}^n$ in $\mathbb{C}^n$ as the parameter becomes complex.

1.1.1 Unitary operators

For θ real, any family induces a family of unitary operators U_θ on $\mathbf{L}^2(\mathbb{R}^n)$; if θ becomes complex, the spectrum of the conjugated Schrödinger operator $\mathbf{P}(\theta) \equiv U_\theta \mathbf{P} U_\theta^{-1}$, $\theta \in \mathbb{R}$, deforms.
Let $g : \mathbb{R}^n \to \mathbb{R}^n$ be a smooth mapping $(C^n, n \geqslant 2)$, with $dg(x) = \mathcal{O}(1)$. Given the family of applications $\phi_\theta(x) : \mathbb{R}^n \to \mathbb{R}^n$ defined as:

$$\phi_\theta(x) = x + \theta g(x), \tag{1.1.1}$$

because $\phi_0(x) = x$, we expect that any application is invertible, if θ sufficiently small. We will denote the derivative $\phi_\theta(x)$ by

$$d\phi_\theta(x) = \mathbf{I}_n + \theta dg(x). \tag{1.1.2}$$

It is invertible for $|\theta| < M_1$,

$$M_1 := (sup_{x\in\mathbb{R}^n}\|dg(x)\|)^{-1}, \tag{1.1.3}$$

where the inverse can be computed explicitly by

$$\sum_n (-1)^n \theta^n (dg)^n. \tag{1.1.4}$$

(The series is absolutely convergent, provided $|\theta|M_1^{-1} < 1$). Thus, by the inverse function theorem, ϕ_θ is invertible on $\mathbb{R}^n$.

Let $\mathcal{S}(\mathbb{R}^n)$ be the Schwartz space of functions that are rapidly decreasing with all their derivatives.

Definition 1. For any $f \in \mathcal{S}(\mathbb{R}^n)$, we define a map U_θ on $\mathcal{S}(\mathbb{R}^n)$ by

$$(U_\theta f)(x) = \sqrt{\mathbf{J}_{\phi_\theta}(x)} f(\phi_\theta(x)),\ \theta \in \mathbb{R}, \tag{1.1.5}$$

where $\mathbf{J}_{\phi_\theta}$ is the Jacobian determinant of the map ϕ_θ.

Proposition 1.1.1. *U_θ maps $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}(\mathbb{R}^n)$. Moreover, for $|\theta| < M_1$, $\theta \in \mathbb{R}$, U_θ extends to a unitary operator on $\mathbf{L}^2(\mathbb{R}^n)$ and the strong limit*

$$s - lim_{\theta\to 0} U_\theta = 1 \tag{1.1.6}$$

(See [HiSi] for the proof).

Example 1. Analytic dilation group:

$$(U_\theta f)(x) = e^{\theta n/2} f(e^\theta x). \tag{1.1.7}$$

Example 2.
Traslation group with direction $\hat{e}$:

$$(U_\theta f)(x) = f(x + \theta\hat{e}). \tag{1.1.8}$$

1.1.2 Complex extension, analytic vectors

Definition 2. Let $\mathcal{A}$ be the linear space of all entire functions $f : \mathbb{C}^n \to \mathbb{C}^n$ such that in any conical region

$$C_\varepsilon \overset{def}{=} \{z \in \mathbb{C}^n; |\mathrm{Im}\ z| \le (1-\varepsilon)|\mathrm{Re}\ z|\}, \tag{1.1.9}$$

for any $\varepsilon > 0$, $\forall k \in \mathbb{N}$

$$\lim_{|z|\to\infty} |z|^k |f(z)| = 0,\ z \in C_\varepsilon. \tag{1.1.10}$$

Remark 1.1.2. $\mathcal{A} \neq \emptyset$; any entire function of the form $f(z) = e^{-\alpha z^2} p(z)$ belongs to $\mathcal{A}$, with p a polynomial, $\alpha > 0$.

Definition 3.
The set of analytic vectors in $\mathbf{L}^2(\mathbb{R}^n)$ is the set of $\psi \in \mathbf{L}^2(\mathbb{R}^n)$ such that $\exists\ f \in \mathcal{A},\ \psi(x) = f(x),\ x \in \mathbb{R}^n$.

Remark 1.1.3.
The set of functions in $\mathcal{A}$ restricted to $\mathbb{R}^n$ forms a dense, linear subset of $\mathbf{L}^2(\mathbb{R}^n)$. Furthermore, for any $f \in \mathcal{A}, f(z) \in \mathbf{L}^2(\mathbb{R}^n)$, for $z \in C_\varepsilon, \forall \varepsilon > 0$.

1.1.3 Spectral deformation

Definition 4. [Type-A families] Let D be a non-empty open subset of $\mathbb{C}$ and suppose that, for each $\theta \in D, \mathbf{P}_\theta$ is a closed operator , with resolvent set $\rho(\mathbf{P}_\theta) \neq \emptyset$. Then the family of closed operators $\mathbf{P}_\theta, \theta \in D$, is said to be Type-$A$ if

i) $D(\mathbf{P}_\theta)$ is independent of θ;

ii) For any $u \in D(\mathbf{P}_\theta), \mathbf{P}_\theta u$ is analytic in θ on D.

Remark 1.1.4. If G is an open bounded set such that $\overline{G} \subset \rho(\mathbf{P}_{\theta_0})$, then

1. $G \subset \rho(\mathbf{P}_\theta)$ for $|\theta - \theta_0|$ sufficiently small.

2. If $\lambda \in G$, the map $D \ni \theta \mapsto (\lambda - \mathbf{P}_\theta)^{-1}$ is analytic in θ for $|\theta - \theta_0|$ sufficiently small.

Namely, $D(\mathbf{P}_\theta) = (\lambda - \mathbf{P}_{\theta_0})^{-1}, (\mathbf{P}_\theta - \mathbf{P}_{\theta_0})(\lambda - \mathbf{P}_{\theta_0})^{-1}$ is closed, everywhere defined, bounded. Thus, for $|\theta - \theta_0| \to 0$, its norm will be smaller than one, then $1 - (\mathbf{P}_\theta - \mathbf{P}_{\theta_0})(\lambda - \mathbf{P}_{\theta_0})^{-1}$ is invertible, for $\lambda \in \rho(\mathbf{P}_\theta)$.

One can easily prove stability of isolated eigenvalues with respect to perturbations given by Type-A families. In addition, if the eigenvalue is non-degenerate, then one can also prove that the corresponding eigenvalue of $\mathbf{P}_{\theta_0}$ is analytic in θ. In general, a degenerate, discrete eigenvalue λ_0, under a perturbation splits into several eigenvalue branches, which converge to λ_0. In the case $\mathbf{P}_{\theta_0}$ self-adjoint, every branch is an analytic function of θ. (See [HiSi])

Let us now suppose:

$(A1)$ There exists a family $\mathcal{U}$ of unitary operators U_θ, $\theta \in D \equiv \{z \in \mathbb{C}/|z| < 1\}$ such that, for $\theta \in D \cap \mathbb{R}, U_\theta$ is unitary, $U_\theta D(\mathbf{P}) = D(\mathbf{P}) \forall \theta \in D$, and $U_0 = 1$. There exists a dense set of vectors $\mathcal{A} \subset \mathcal{H}$ such that

- **i)** the map $\mathcal{A} \times D \ni (\psi, \theta) \mapsto U_\theta \psi$ is analytic on D with values in $\mathcal{H}$;
- **ii)** For $\theta \in D, U(\theta)$ is dense in $\mathcal{A}$.

$(A2)$ Define, for $\theta \in D \cap \mathbb{R}$, a family of unitary equivalent operators $\mathbf{P}(\theta) \equiv U_\theta \mathbf{P} U_\theta^{-1}$. Let assume that the map $D \ni \theta \mapsto \mathbf{P}(\theta)$ is analytic of type-A.

The family $\mathcal{U}$ satisfying $(A1)$ and $(A2)$ is called *Spectral deformation family* for $\mathbf{P}$. The dense set $\mathcal{A}$ of vectors is said to be of "analytic vectors" for U_θ. The condition (A2) can be relaxed, it is sufficient to state the analiticity of the resolvent of $\mathbf{P}_\theta$ in θ.

Let us consider the spectrum $\sigma(\mathbf{P}_\theta)$ of $\mathbf{P}_\theta$. In general is a closed subset of $\mathbb{C}$ that may have a nonempty interior. Moreover, $\mathbf{P}_\theta$ may have complex eigenvalues that have no counterpart in $\sigma(\mathbf{P})$.

Example 3 (dilation analyticity)**.**
Consider $\mathbf{P}_{\theta_0} = -\Delta$ on $\mathbf{L}^2(\mathbb{R}^n)$ and recall that $\sigma_{ess}(\mathbf{P}_0) = [0, \infty)$.
If $f \in \mathcal{S}(\mathbb{R}^n)$, U_θ is defined by (1.1.7). It is easy to check that $\{U_\theta; \theta \in \mathbb{R}\}$ forms a one-parameter unitary group, and that $U_\theta D(\mathbf{P}_0) = D(\mathbf{P}_0)$, $\theta \in \mathbb{R}$.
Consider U_θ acting on the set of analytic vectors (dense $\mathbf{L}^2(\mathbb{R}^n)$) of the type

$$\psi(z) = p(z) e^{-\alpha z^2}, \tag{1.1.11}$$

cor $\alpha > 0, z \in \mathbb{C}^n$, p polynomial. Then, as long as conditions on the positivity of $Re(e^{2i\theta})$ hold, the function $U_\theta \psi \in \mathbf{L}^2(\mathbb{R}^n)$, and the map

$$(\theta, \psi) \in D \times \mathcal{A} \mapsto U_\theta \psi \tag{1.1.12}$$

is analytic on $\mathbf{L}^2$. Moreover,

$$\mathbf{P}_0(\theta) = e^{-2\theta} \Delta = e^{-2\theta} \mathbf{P}_0. \tag{1.1.13}$$

After a change of coordinates, by replacing $\theta \to i\theta$ and considering from now on θ complex, we have:

$$\sigma_{ess} H_0(i\theta) = e^{-2i\theta} \overline{\mathbb{R}^+}. \tag{1.1.14}$$

Thus the essential spectrum of $\mathbf{P}_0$ will rotate about the origin through an angle of -2θ, as result of the spectral deformation.

Let us consider in general the action of a spectral deformation family $\mathcal{U}$ on a set $\mathcal{A}$ of analytic vectors.

Proposition 1.1.5. *(see [HiSi]) Let $\mathcal{U}$ be a family of spectral deformation related to the smooth vector field g, that satisfies*

$$\sup_{x\in\mathbb{R}^n} \|dg(x)\| \leq 1. \tag{1.1.15}$$

Set

$$D_0 = \{\theta \in \mathbb{C}; |\theta| < \theta_0\}, \tag{1.1.16}$$

where $\theta_0 << 1$. Thus,

(i) *The map $D_0 \times \mathcal{A} \ni (\theta, f) \mapsto U_\theta f$ is an analytic function with values in $\mathbf{L}^2$;*

(ii) *For any $\theta \in D_0, U_\theta \mathcal{A}$ is dense in $\mathbf{L}^2$.*

We can now apply the previous theory to study the Schrödinger operator $\mathbf{P} = -h^2\Delta + V(x)$. Assume that $h > 0$ and g satisfies condition (1.1.15), $g(x) = x$ for $|x| \gg 1$, and that $\mathbf{P}$ is self-adjoint with domain $D(\mathbf{P}) = H^2(\mathbb{R})$.
Let D_0 be the disk defined in (1.1.16), and consider, for $\theta \in D_0 \cap \mathbb{R}$, the family of unitary equivalent operators

$$\mathbf{P}(\theta) \equiv U_\theta \mathbf{P} U_\theta^{-1} = p_\theta^2 + V_\theta, \tag{1.1.17}$$

where

$$p_\theta^2 = U_\theta p^2 U_\theta^{-1}, \quad p_j \equiv -ih\frac{\partial}{\partial x_j}, \tag{1.1.18}$$

and

$$V_\theta = U_\theta V U_\theta^{-1}. \tag{1.1.19}$$

The operator p_θ^2 can be computed explicity, and it comes out:

$$p_\theta^2 \equiv \left((d\phi_\theta\,(x))^{-1} \cdot p\right)^2 + ha(x) \cdot p \tag{1.1.20}$$

($a(x) \cdot p$ is a first order operator 1 with compact supported coefficients).

Proposition 1.1.6. *(see, e.g. [HiSi], Prop. 18.1)*
The family of operators p_θ^2, $\theta \in D_0$, defined in (1.1.18) is a type-A analytic family of operators with domain $D(p_\theta^2) = H^2(\mathbb{R}^n)$.

Proposition 1.1.7. *(see [HiSi], Prop. 18.2) Let p_θ^2 be defined as in (1.1.18). Then:*

$$\sigma_{ess}(p_\theta^2) = \{z \in \mathbb{C}; \arg z = -2\arg(1+\theta)\}, \tag{1.1.21}$$

for any $\theta \in D_0$.

We consider the potential V. Let C_ε^R be the *truncated cone* obtained from C_ε in (1.1.9) with the additional condition that there exists $R > 0$ such that $\|\mathrm{Re}\, z\| > R$. We already know, for $\theta \in D_0$ and $\|x\| > R$, $R \gg 1$, that the image of $\phi_\theta(x)$ is contained in C_ε.
We need then additional assumptions on the potential V since:

1. The modified potential $V \circ \phi_\theta$ has to be extended, for $\theta \in D_0$ as p^2-relatively compact operator;

2. We want to compute $\sigma_{ess}(\mathbf{P}(\theta))$, starting from the previous proposition.

Definition 5. We call a real valued function V on $\mathbb{R}^n$ for a spectral deformation family $\mathcal{U}$ *admissible potential* if :

$(V1)$ V is relatively p^2-compact;

$(V2)$ V is the restriction to $\mathbb{R}^n$ that is analytic on the truncated cone C_ε^R, for any $\varepsilon > 0$ and some $R > 0$ sufficiently large.

If V satisfies both conditions, then $V \circ \phi_\theta$ extends to $\theta \in D_0$ as an analytic, relatively p_θ^2-compact operator.

Lemma 1.1.8. *Let V satisfy ($V1$) and ($V2$). Then the self-adjoint operator $\mathbf{P}(\theta) = p_\theta^2 + V_\theta$, defined for $\theta \in D_0 \cap \mathbb{R}^n$, extends to an analytic type-A family of operators on D_0 with domain $H^2(\mathbb{R}^n)$.*

Theorem 1.1.9. *Let $\mathcal{U}$ be a spectral deformation family for the Schrödinger operator $\mathbf{P} = -h^2\Delta + V$, where V satisfies ($V1$) and ($V2$). Then for any $\theta \in D_0$,*

$$\sigma_{ess}(\mathbf{P}(\theta)) = \{z \in \mathbb{C}; \arg z = -2\arg(1+\theta)\}. \tag{1.1.22}$$

To prove (1.1.9) we recall the Weyl Theorem (1.1.10) and we refer to the subsequent remark:

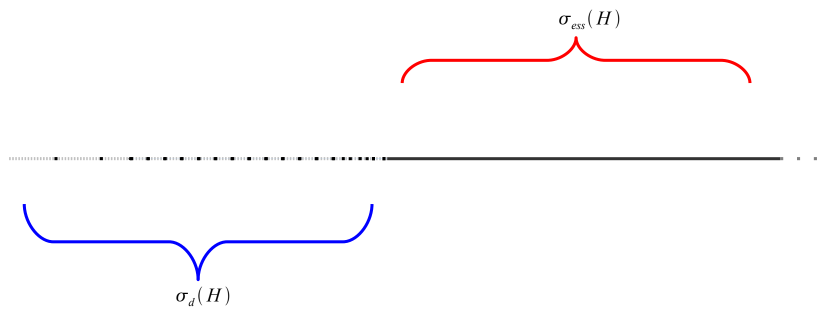


Figure 1.1: Spectrum of Schrödinger operator

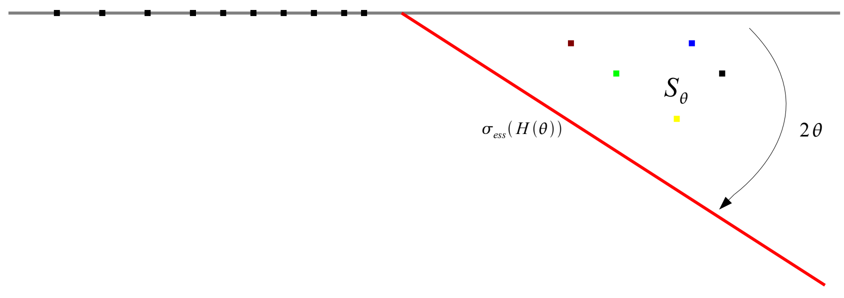


Figure 1.2: Spectrum of deformed Schrödinger operator

Theorem 1.1.10. *[Weyl theorem]*
Let A be a closed operator on a Hilbert space $\mathcal{H}$, and B a relatively A-compact operator. Then:

$$\sigma_{ess}(A) = \sigma_{ess}(A + B). \tag{1.1.23}$$

Remark 1.1.11. (Distorsion on the Laplacian)
By computing the essential spectrum of the distorted operator p_θ^2, we focus on the term coming out from the complex distorsion of $(d\phi_\theta)^{-1}$. Thanks to the assumptions (1.1.1, 1.1.2, 1.1.3), we find an expression of the type

$$(d\phi_\theta)^{-1} = e^{-i\theta} + M_0, \tag{1.1.24}$$

where M_0 is a compact supported matrix.
Substituting in (1.1.20) we obtain

$$p_\theta^2 = e^{-2i\theta}p^2 + \langle A(x)\cdot p, p\rangle + ha(x)\cdot p, \tag{1.1.25}$$

where $ha(x)\cdot p$ is relatively compact, and $A(x)$ is a compact supported matrix. Then, applying the theorem (1.1.10) in this case we find:

$$\sigma_{ess}(p_\theta^2) = \sigma_{ess}\big(e^{-2i\theta}p^2 + \langle A(x)\cdot p, p\rangle\big). \tag{1.1.26}$$

Set $B_0 \equiv e^{-2i\theta}$, $\quad \langle A(x)\cdot p, p\rangle \equiv b(x,p)$, $\quad B \equiv B_0 + b(x,p)$. In order to apply again theorem (1.1.10) we act on the resolvents: instead of check for information about compactness of $b(x,p) \equiv B - B_0$, we evaluate the resolvents on a certain element which does not belong to the spectrum, for example on $-i \notin \sigma(B)$:

$$\begin{gathered}
(B+i)^{-1} - (B_0+i)^{-1} = (B+i)^{-1}(I - (B+i)(B_0+i)^{-1}) = \\
(B+i)^{-1}\big((B_0+i)(B_0+i)^{-1} - (B+i)(B_0+i)^{-1}\big) = \\
(B+i)^{-1}\big[(B_0+i) - (B+i)\big](B_0+i)^{-1} = \\
(B+i)^{-1}(B_0 - B)(B_0+i)^{-1} = \\
-(B+i)^{-1}b(x,p)(B_0+i)^{-1}.
\end{gathered}$$

The previous operator is compact from L^2 to L^2:

- The map $(B_0)^{-1} : L^2 \to H^2$ is bounded.
- By composition on the RHS of b with a cut-off function χ, $\chi(x) = 1$ for $x \in SuppA(x) := K$, with $C \gg 1$, we obtain $b(x,p) = L(x,p)\chi(x)$, thus $\chi(x)(B_0+i)^{-1} : L^2 \to H_k^2$ is compact. (Where H_K^2 is the set of compactly supported functions on K).

- The identity $I : H^2_K \to L^2$ (by Sobolev theorem) is compact.
- The map $(B+i)^{-1}b$ is bounded on L^2.
  Summing up:

$$L^2 \overset{(B_0+i)^{-1}}{\longrightarrow} H^2 \overset{\chi_K}{\longrightarrow} H^2_K \overset{I}{\longrightarrow} L^2 \overset{(B+i)^{-1}b}{\longrightarrow} L^2 \tag{1.1.27}$$

Therefore $(B+i)^{-1} - (B_0+i)^{-1}$ is compact, and applying theorem (1.1.10) (by substituting $A+B = (B+i)^{-1}, A = (B_0+i)^{-1}$), the following equality holds:

$$\sigma_{ess}((B+i)^{-1}) = \sigma_{ess}((B_0+i)^{-1}). \tag{1.1.28}$$

Now we apply the *Spectral Mapping Theorem* (Theorem 1.e, Cap. VII [ReSi]):

$$\sigma_{ess}(B+i) = \sigma_{ess}(B_0+i), \tag{1.1.29}$$

thus

$$\sigma_{ess}(B) = \sigma_{ess}(B_0). \tag{1.1.30}$$

The essential spectrum of p^2_θ is then exactly $e^{-2i\theta}\sigma_{ess}(p^2)$.

1.2 Resonances for the Schrödinger operator

The theory developed by Aguilar, Balslev, Combes e Hunziker since 1970, identify the resonances with the eigenvalues of the deformed hamiltonian $\mathbf{P}_\theta$ in the lower complex half-plane. The resonances do not depend on θ and g, and they are associated with the poles of the meromorphic extension from the upper complex half-plane of the resolvent $R_{\mathbf{P}}(z)$. In order to prove the existence of such continuation we operate an explicit construction assuming appropriate conditions.

Theorem 1.2.1. *Let* $\mathbf{P}$ *be a self-adjoint Schrödinger operator with spectral deformation family* $\mathcal{U}$ *satisfying (A1) and (A2) with set of analytic vectors* $\mathcal{A}$ *, and such that* $\sigma_{ess}(\mathbf{P}) = [0,\infty)$, $\sigma_d(\mathbf{P}) \subset (-\infty, 0]$.
We consider a connected open set $\Omega \subset \{z \in \mathbb{C}; \mathrm{Re}\, z > 0\}$, *with* $\Omega^+ \equiv \Omega \cap \mathbb{C}^+ \neq \emptyset$, $\Omega^- \equiv \Omega \cap \mathbb{C}^- \neq \emptyset$ *(setting* $\mathbb{C}^\pm = \{\pm\mathrm{Im}\, z \geq 0\}$*). For any* $\varepsilon > 0$ *there exists a subset* $\Omega^-_\varepsilon \subset \Omega^-$, *such that, for some* $\theta \in D_\varepsilon \equiv \{\theta \in D_0; \mathrm{Im}\, \theta > \varepsilon\}$, *we have* $\sigma_{ess}(\mathbf{P}(\theta)) \cap \Omega^-_\varepsilon = \emptyset \quad \forall \varepsilon > 0$. *Then:*

1. *For* $f, g \in \mathcal{A}$, *the function*

$$F_{fg}(z) \equiv \langle f, R_{\mathbf{P}}(z) g \rangle, \tag{1.2.1}$$

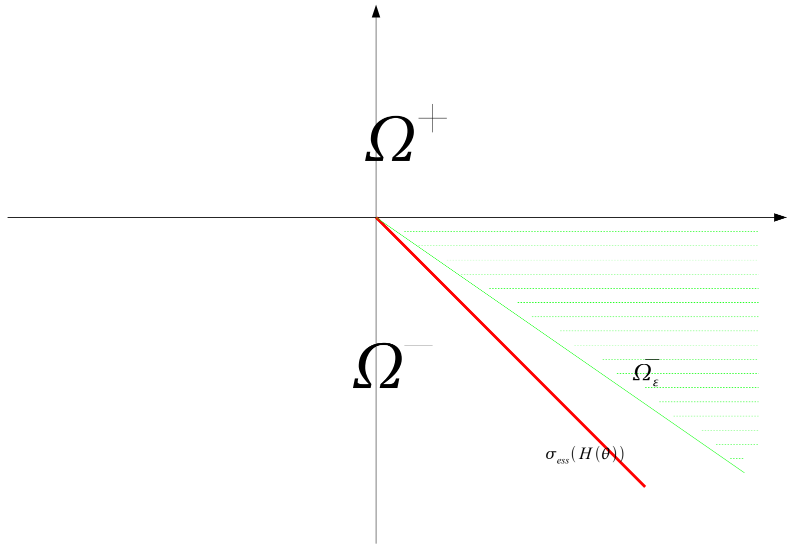


Figure 1.3: Spectrum of a deformed family

defined for $\operatorname{Im} z > 0$*, has a meromorphic continuation across* $\sigma_{ess}(\mathbf{P}) = \overline{\mathbb{R}^+}$ *in* Ω_ε^- $\forall \varepsilon > 0$.

2. *The poles of the continuation of* $F_{fg}(z)$ *into* Ω_ε^- *are eigenvalues of all the operators* $\mathbf{P}_\theta, \theta \in D_\varepsilon$ *, such that* $\sigma_{ess}(\mathbf{P}_\theta) \cap \Omega_\varepsilon^- = \varnothing$.

3. *These poles are independent of* $\mathcal{U}$ *: let* $\mathcal{V}$ *be a spectral deformation family for* $\mathbf{P}$*, with a set of analytic vectors* $\mathcal{A}_\mathcal{V}$ *satisfying the previous assumptions and such that* $\mathcal{A} \cap \mathcal{A}_\mathcal{V}$ *is dense. Then the eigenvalues of* $\widetilde{\mathbf{P}_\theta} \equiv V_\theta \mathbf{P} V_\theta^{-1}$, $\theta \in D_\varepsilon$*, in* Ω_ε^-*, are the same as those of* $\mathbf{P}_\theta$ *in this region.*

Proof. Let us fix $z \in \mathbb{C}^+$.

For θ real U_θ is invertible, and $U_\theta^{-1} = U_\theta^*$. Therefore we can write

$$F_{fg}(z) \equiv \langle U_\theta f, (U_\theta R_\mathbf{P}(z) U_\theta^{-1}) U_\theta g \rangle. \tag{1.2.2}$$

By condition $(A1)$ $\theta \in D \mapsto U_\theta f, U_\theta g$ are analytic maps and the following equality holds:

$$U_\theta R_\mathbf{P}(z) U_\theta^{-1} = R_{\mathbf{P}_\theta}(z). \tag{1.2.3}$$

By assumption $(A2)$ the map $\theta \in D \mapsto R_{\mathbf{P}_\theta}(z)$ is analytic if $z \notin \sigma(\mathbf{P}(\theta))$. Furthermore, for $\theta \in D \cap \mathbb{R}$, (where $\theta \equiv \overline{\theta}$), we have:

$$\theta \in D \longrightarrow F_{fg}(z, \theta) \equiv \langle U_{\overline{\theta}} f, R_{\mathbf{P}(\theta)}(z) U_\theta g \rangle. \tag{1.2.4}$$

This map is analytic , well defined for $\theta \in \mathbb{C}$, we can then extend for θ in D_ε and z in $\Omega_\varepsilon^+ \subset \Omega^+$. We fix $\theta \in D_\varepsilon$; $F_{fg}(z)$ can be meromorphically continued in z, from $\{\mathrm{Im}\, z > 0\}$ into $\mathbb{C}\backslash\sigma_{ess}(\mathbf{P}(\theta))$. The identity principle for meromorphic functions permits us, since

$$F_{fg}(z,\theta) \equiv F_{fg}(z) \text{ for } \mathrm{Im}\, z > 0, \tag{1.2.5}$$

to state the existence of a meromorphic function on $\Omega_\varepsilon^- \cup \Omega_\varepsilon^+$, that coincides with $F_{fg}(z)$ on Ω_ε^+. This function is the extension into Ω_ε^-.

The meromorphic continuation of $F_{fg}(z)$ in Ω_ε^- is given by the matrix elements of $R_{\mathbf{P}_\theta}(z)$ computed in the states f_θ e g_θ, which denote the continuation of $U_\theta f$ e $U_\theta g$. Condition $(A1)$ states that such vectors in $U_\theta\mathcal{A}$, $\theta \in D_0$, are dense. Therefore, if $\mathbf{P}_\theta$ has an eigenvalue at $\lambda_\theta \in \Omega_\varepsilon^-$, $F_{fg}(z)$ will have a pole there; vice versa, if $F_{fg}(z)$ has a pole at λ_θ, then it must be an eigevalue of $\mathbf{P}_\theta$.

We conclude that the poles of the continuation of F_{fg} in $\overline{\Omega_\varepsilon^-}$ are independent of θ. In fact, if $z_i \in \overline{\Omega_\varepsilon^-}$ is a pole for $F_{fg}(z,\theta)$, due to uniqueness of the identity principle for meromorphic functions, it is a pole for $F_{fg}(z,\theta')$, since they both coincide with $F_{fg}(z)$ on Ω_ε^+. Thus the eigenvalues of $\mathbf{P}_\theta, \theta \in D_\varepsilon$, are the same of $\mathbf{P}(\theta')$, $\theta' \in D_\varepsilon$, supposing z_i away from $\sigma_{ess}(\mathbf{P}(\theta'))$. The last statement of the theorem comes again from the uniqueness . □

Corollary 1.2.2. *Under the same hypothesis of the theorem:*

(i) $\sigma_d(\mathbf{P}(\theta)) \cap \Omega_\varepsilon^+ = \emptyset$, $\theta \in D_\varepsilon$.

(ii) *any* $\lambda \in \sigma_d(\mathbf{P}_\theta)$, $\theta \in D_\varepsilon$, *is independent of* θ, *provided* $\lambda \notin \sigma_{ess}(\mathbf{P}(\theta))$.

(iii) *If* λ *is an eigenvalue of* $\mathbf{P}$, *then* $\lambda \in \sigma_d(\mathbf{P}(\theta))$ *for* $\theta \in D_\varepsilon$.

Proof. **(i)** $F_{fg}(z,\theta) = F_{fg}(z)$ for $\theta \in D_\varepsilon$, $\mathrm{Im}\, z > 0$. $\mathbf{P}$ is self-adjoint; if $\sigma_d(\mathbf{P}_\theta) \cap \{\mathrm{Im}\, z > 0\} \neq 0$ we would have an eigenvalue for $\mathbf{P}_\theta$, thus a pole. Therefore $\mathbf{P}$ would have a complex eigenvalue $z \in \{\mathrm{Im}\, z > 0\}$.

(ii) The continuation $F_{fg}(z)$ is unique and independent of θ. Hence as $\lambda \in \sigma_d(\mathbf{P}(\theta))$ is a pole of this continuation for some $f, g \in \mathcal{A}$, it is independent of θ.

(iii) Let suppose $\lambda \in \sigma_d(\mathbf{P})$. Let

$$\Pi = \frac{1}{2\pi i}\oint_\Gamma R_{\mathbf{P}}(z)dz \tag{1.2.6}$$

be the orthogonal projection of $\mathbf{P}$, where Γ is a closed contour about λ. There exist $\varphi, \psi \in L^2$ such that $\langle\varphi, \Pi\psi\rangle \neq 0$. Then, by density of $\mathcal{A}$, we can find

$f, g \in \mathcal{A}$ with

$$\langle f, \Pi g \rangle \neq 0. \tag{1.2.7}$$

If λ is isolated from $\sigma_{ess}(\mathbf{P}(\theta))$, for $\theta \in D_\varepsilon$,

$$\langle f, \Pi g \rangle = \langle U_{\overline{\theta}} f, \Pi_\theta U_\theta g \rangle \tag{1.2.8}$$

holds, where

$$\Pi_\theta = U_\theta \Pi U_\theta^{-1} = \frac{1}{2\pi i} \oint R_{\mathbf{P}(\theta)}(z) dz \tag{1.2.9}$$

is the spectral projection of $\mathbf{P}_\theta$ on $Int(\Gamma)$. The matrix element has continuation for $\theta \in D_\varepsilon$.

Then $Int(\Gamma) \cap \sigma_d(\mathbf{P}_\theta) = \emptyset$ for any contour Γ about λ. Thus $\lambda \in \sigma_d(H(\theta))$.

□

It follows from the previous theorem and corollary, that the set $Res(\mathbf{P})$ of resonances of $\mathbf{P}$, in the sector Ω_ε^- can be given by:

$$Res(\mathbf{P}) \cap \Omega_\varepsilon^- = \bigcup_{\theta \in D_\varepsilon} \sigma_d(\mathbf{P}_\theta) \cap \Omega_\varepsilon^-. \tag{1.2.10}$$

Thus we have the following definition:

Definition 6. The quantum resonances of a Schrödinger operator $\mathbf{P}$ associated with a dense set of analytic vectors $\mathcal{A}$, are the poles of the meromorphic continuation of all matrix elements

$$\langle f, R_{\mathbf{P}}(z) g \rangle, f, g \in \mathcal{A}, \tag{1.2.11}$$

from $\{z \in \mathbb{C}; \text{Im } z > 0\}$ to $\{z \in \mathbb{C}; \text{Im } z < 0\}$.

1.3 Distorsion of pseudodifferential operators

Let $\mathbf{A} = Op_h(a)$ be a pseudodifferential operator, with symbol $a \in \mathcal{S}_{3n}(\langle \xi \rangle^m)$. We assume that there exists δ such that a is holomorphic in

$$\Gamma := \big\{ |\text{Re } x| > R_0, |\text{Im } x| < \delta |\text{Re } x| \big\} \times \big\{ |\text{Re } y| > R_0, |\text{Im } y| < \delta |\text{Re } y| \big\} \times \\ \big\{ |\text{Im } \xi| < \delta \langle \text{Re } \xi \rangle \big\},$$

and $\partial^\alpha a = \mathcal{O}(\langle \text{Re } \xi \rangle^m)$, where $\delta > 0$, $R_0 \gg 1$.

We want to obtain an expression of the type

$$U_\theta \mathbf{A} U_\theta^{-1} = Op_h^W\big(a_\theta(x, \xi)\big), \tag{1.3.1}$$

where the symbol of the distorted operator a_θ has similar properties of a , in order to define resonances. We consider

$$\mathbf{A}u(x) = \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} e^{-i(x-y)\xi/h}a(x,y,\xi)u(y)dyd\xi, \tag{1.3.2}$$

and applying distorsion with $\theta \in \mathbb{R}$, setting $\frac{1}{(2\pi h)^n} \equiv \alpha$, $\phi_\theta(x) \equiv \phi$, we obtain

$$U_\theta \mathbf{A} U_\theta^{-1} = \alpha \int e^{-i(x+\theta g(x)-y)\xi/h} a(x+\theta g(x), y, \xi)u(y)J_\phi^{1/2}J_{\phi^{-1}}dyd\xi = \tag{1.3.3}$$

(by changing integration variable $y \to z + \theta g(z)$)

$$= \alpha \int e^{-i(x-z+\theta(g(x)-g(z)))\xi/h} a(x+\theta g(x), z+\theta g(z), \xi)u(z+\theta g(z))\times$$

$$\times J_\phi^{1/2}J_{\phi^{-1}}J_\phi^{1/2}dzd\xi.$$

The scalar product in the exponent becomes

$$\big[x - z + \theta(g(x) - g(z))\big]\cdot\xi = \sum_{i,j}(x_i - z_i)\big\{\delta_{ij} + \theta\int_0^1 \frac{dg_j}{dx_j}(tx + (1-t)z)\big\}\xi_j =$$

$$(x-z)\big(I + \theta F(x,z)\big)\cdot\xi = (x-z)\cdot {}^t(I + \theta F(x,z))\xi,$$

where $F(x,z)$ is a bounded function, given by the expression

$$\big(F_{ij}(x,z)\big) = \int_0^1 \frac{dg_j}{dx_i}\big(tx + (1-t)z\big)dt. \tag{1.3.4}$$

By a further change of variable

$$\eta = {}^t(I + \theta F(x,z))\xi, \tag{1.3.5}$$

we obtain

$$\xi = {}^t(I + \theta F(x,z))^{-1}\eta, \Rightarrow d\xi = \det(I + \theta F(x,z))^{-1}d\eta, \tag{1.3.6}$$

and by substitution in (1.3):

$$= \alpha \int e^{-i(x-z)\eta/h} a\big(x+\theta g(x), z+\theta g(z), {}^t(I+\theta F(x,z))^{-1}\eta\big)u(z+\theta g(z))\cdot$$

$$J_\phi^{1/2}(x)J_{\phi^{-1}}J_\phi^{1/2}(z)\det\big(I+\theta F(x,z)\big)^{-1}dzd\eta =$$

$$= \alpha \int e^{-i(x-y)\xi/h}\tilde{a}_\theta(x,y,\xi)u(y)dyd\xi, \tag{1.3.7}$$

where $\tilde{a}_\theta(x,y,\xi)$ is obtained denoting the new variables $z \to y, \eta \to \xi$, from

$$a\big(x+\theta g(x), z+\theta g(z), {}^t(I+\theta F(x,z))^{-1}\eta\big)J_\phi^{1/2}(x)J_{\phi^{-1}}J_\phi^{1/2}(z)\det\big(I+\theta F(x,z)\big)^{-1}. \tag{1.3.8}$$

This symbol is well defined, of order m, $g(x) \equiv x$ for $|x| \gg 1$, and all the determinants are bounded. Now we can extend θ to a complex value and consider the pseudodifferential operator

$$\mathbf{A}_\theta \equiv U_\theta \mathbf{A} U_\theta^{-1} = Op_h^W(a_\theta), \tag{1.3.9}$$

where the new symbol has been changed by Weyl quantization thanks to the theorem 2.7.1 in ([Ma2]).

Remark 1.3.1. If $m = 0$ and $\partial^\alpha a \to 0$ for $(x, y, \xi) \to \infty$ in $\Gamma \cap \{|x - y| < \delta|x|\}$, then $\mathbf{A}_\theta$ is compact.

Remark 1.3.2. In particular, this is true if we consider operators of the type $\mathcal{A} = Op_h^0(a)$ (with left-quantization), or as $\mathcal{A} = Op_h^1(a)$ (right-quantization), $a \in \mathcal{S}_{2n}(1)$ and holomorphic in $\{|\text{Re } x| > 0, |\text{Im } x| < \delta|\text{Re } x|\} \times \{|\text{Im } \xi < \delta\langle\text{Re } \xi\rangle\}$. By Weyl quantization we need to assume a holomorphic in $\{|\text{Im } x| < \delta\langle\text{Re } x\rangle\} \times \{|\text{Im } \xi| < \delta\langle\text{Re } \xi\rangle\}$.

We consider now a matrix operator of the type

$$P = -h^2 \Delta I_N + V + hOp_h(a), \tag{1.3.10}$$

such that

- $V = \big(V_{ij}(x)\big)_{1 \le i,j \le N}, \quad V_{ij} \in \mathcal{S}_n(1);$
- $a = \big(a_{ij}(x, y, \xi)\big)_{1 \le i,j \le N}$, where the symbols a_{ij} satisfy the assumptions of previous paragraph (1.3), $m = 1$;
- $\forall \alpha \in \mathbb{N}^{2n}, \quad \langle\xi\rangle^{-1}\partial^\alpha a \longrightarrow 0$ for $|x| \to \infty$, uniformly with respect to (y, ξ) in $\Gamma \cap \{|x - y| < \delta|x|\}$ (Compactness assumption).

Under the previous assumptions there exists a distorted operator P_θ, $\theta \in i\mathbb{R}^+$, $\theta \ll 1$, of the form

$$P_\theta = U_\theta(-h^2\Delta)U_\theta^{-1} + V_\theta + h\mathcal{A}_\theta, \tag{1.3.11}$$

where $\mathcal{A}_\theta$ is Δ-compact.

By applying the general consideration of (1.2) to P_θ we can define the resonances of P as the complex eigenvalues of P_θ.

1.4 Example: the shape resonances

This model was developed by Gamov, Gurney and Condon (see [Ga], [GC]) to describe the decay of instable atomic nuclei, with emission of alpha particles. The nucleus is modeled as a potential barrier of finite length, that "traps" the alpha particle. The wave function is at first localized in the potential well, oscillating between the barriers. Since their thickness is finite, the wave function will penetrate them, and the probability to escape to infinity for the particle is not zero. We consider the Schrödinger operator

$$P = -h^2\Delta + V(x) + hA(x, hD_x), \tag{1.4.1}$$

where V has the "shape" of potential barrier with finite thickness, determined by the semiclassical parameter h, and A is a pseudo-differential operator as in section (1.3). The life-time of the particle is controlled by the properties of V and h; If $\rho = E - i\Gamma$, $\Gamma > 0$ is the associated resonance, the particle lives $\frac{1}{|\Gamma|}$. The assumptions on the potential are:

(**V**1) $V \in C^\infty$ real valued; there exists a compact set $K \subset \mathbb{R}^n$ such that V is analytic on $K^C = \mathbb{R}^n \backslash K$, and can be holomorphically extended in a sector:

$$D_0 = \big\{x \in \mathbb{C}^n; |\text{Im } x| < \delta |\text{Re } x|, \text{Re } x \in K^C\big\} \tag{1.4.2}$$

for some $\delta > 0$. Additionally $V(x) \to 0$ for $|\text{Re } x| \to \infty$.

(This assumption permits us to define as usual the resonances near the real axis. If u_θ is an eigenvalue of P_θ, it can be extended holomorphically on D_0, such that $u_\theta = U_{i\theta}u$. Such u's are called resonant states.)

(**V**2) There exists an open, bounded domain $\mathcal{O}$, with smooth boundary, such that V has a non degenerate minimum in $x_0 = 0$, i.e. $Hess\big(V(x_0)\big)$ is positive defined, and we assume for simplicity $V(0) = 0$.

(**V**3) (non-trapping) For any $(x, \xi) \in p^{-1}(0)$

$$|\exp tH_p(x, \xi)| \longrightarrow \infty \quad \text{ as } t \to \infty, \tag{1.4.3}$$

where $p(x, \xi) := \xi^2 + V(x)$ is the symbol of P, and $H_p := (\nabla_\xi p, -\nabla_x p)$ is the Hamiltonian field of p.

The classical forbidden region is defined as $\text{CFR}(E) \equiv \big\{x \in \mathbb{R}^n; V(x) > E\big\}$.

Assumption (**V**1) implies that CFR has compact closure. If it is non-empty, then the complementary set in $\mathbb{R}^n$ consists of two closed and disconnected regions, the potential well $W(E)$ (compact, containing the origin), and the unlimited region outside, $\Sigma(E)$. V represents the geometrical situation of a "*well in an island*", that originally describes the shapes resonances; in particular, the assumption ($\mathbf{V}2$) describes the shape of $V(x)$ in the island.

A very accurate study of this argument was made by Helffer e Sjöstrand in [HeSj2] in the global analytic case with $A = 0$, whereas for the case with analyticity only at infinity one can refer to [FLM] (for $A = 0$).

The method (which can be extended to the case $A = 0$) consists in extending the solutions (WKB-method) from the bottom of the well to a neighborhood of Γ, and estimate the difference with the resonant state. With a non-trapping condition for V, it becomes an admissible potential for P, and one can apply analytical distortion (with a Type-A analytical family).

If e_j denotes the j^{th} eigenvalue of the harmonic oscillator

$$-\Delta + \frac{1}{2}\langle V''(0)x, x\rangle, \tag{1.4.4}$$

one can find that, for any j, there exists a resonance:

$$\rho_j = h\big(e_j + a(0,0,0)\big) + \mathcal{O}(h^2), \tag{1.4.5}$$

where the asymptotic expansion is given by $\rho_j \sim \sum_{k\geq 2} \rho_{jk} h^{\frac{k}{2}}, \quad \rho_{jk} \in \mathbb{R}$.

Furthermore, one can estimate $|\mathrm{Im}\ \rho_j| = \mathcal{O}\big(e^{-S/h}\big)$, with $S > 0$ geometrical constant concerning the tunnel effect.

Chapter 2

The shape resonances

2.1 Notations and assumptions

We study the spectral properties near energy 0 of the semiclassical Schrödinger operator,

$$P := -h^2\Delta + V(x)$$

on $L^2(\mathbb{R}^n)$, where $x = (x_1, \dots, x_n)$ is the current variable in $\mathbb{R}^n$ $(n \geq 1)$, $h > 0$ denotes the semiclassical parameter, and V represents the potential energy.

We assume,

Assumption 1. *The potential V is smooth and bounded on $\mathbb{R}^n$, and it satisfies,*

- $\{V \leq 0\} = U \cup \mathcal{M}$ *where U is compact and connected, $\mathcal{M}$ is closed, and $U \cap \mathcal{M} = \emptyset$;*
- *V has a strictly negative limit $-L$ as $|x| \to \infty$.*

This typically describes the situation where so-called shape resonances appear. In order to be able to define such resonances, we assume,

Assumption 2. *The potential V extends to a bounded holomorphic functions near a complex sector of the form, $\mathcal{S}_\delta := \{x \in \mathbb{C}^n\,;\, |\mathrm{Im}\, x| \leq \delta|\mathrm{Re}\, x|\}$, with $\delta > 0$. Moreover V tends to its limit at ∞ in this sector.*

We also assume,

Assumption 3. *$E = 0$ is a non-trapping energy for V above $\mathcal{M}$:*

The fact that 0 is a non-trapping energy for V above $\mathcal{M}$ means that, for any $(x,\xi) \in p^{-1}(0)$ with $x \in \mathcal{M}$, one has $|\exp tH_p(x,\xi)| \to +\infty$ as $|t| \to \infty$, where $p(x,\xi) := \xi^2 + V(x)$ is the symbol of P, and $H_p := (\nabla_\xi p, -\nabla_x p)$ is the Hamilton vector field of p. It is equivalent to the existence of a function $F \in C^\infty(\mathbb{R}^{2n};\mathbb{R})$, supported near $\{p = 0\} \cap \{x \in \mathcal{M}\}$, that satisfies,

$$H_p F(x,\xi) > 0 \text{ on } \{p(x,\xi) = 0\}. \tag{2.1.1}$$

In particular, $\mathcal{M}$ has a smooth boundary: since the only $\xi \in \mathbb{R}^n$ such that $p(x,\xi) = 0$ is 0, and $H_p = -\nabla V(x) \cdot \partial/\partial\xi$, it implies that $\nabla V(x) \neq 0$ on $\partial\mathcal{M}$.

We denote by d_V the Lithner-Agmon distance associated with V, that is, the pseudo-distance associated with the pseudo-metric $\max(0, V(x))dx^2$.

In the rest of the chapter we set,

$$S_0 := d_V(U, \mathcal{M}).$$

Thanks to our assumptions, we necessarily have $S_0 > 0$.

2.2 Resonances

In the previous situation, the essential spectrum of P is $[-L, +\infty)$. The resonances of P can be defined by using a complex distortion as in chapter 1: Let $g \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$ such that $g(x) = x$ for $|x|$ large enough. For $\theta \neq 0$ small enough, we define the distorted operator P_θ as the value at $\nu = i\theta$ of the extension to the complex of the operator $U_\nu P U_\nu^{-1}$ which is defined for ν real, and analytic in ν for ν small enough, where U_ν is defined by (1.1.5). By using the Weyl Perturbation Theorem (1.1.10), one can also see that the essential spectrum of P_θ is given by,

$$\sigma_{ess}(P_\theta) = e^{-2i\theta}\mathbb{R}_+ - L.$$

It is also well known that, when θ is positive, the discrete spectrum of P_θ satisfies,

$$\sigma_{disc}(P_\theta) \subset \{\text{Im } z \leq 0\}.$$

Then, those eigenvalues of P_θ that are located in the complex sector $\{\text{Re }(z) > L\,;\, -2\theta < \arg(z + L) \leq 0\}$ are called the resonances of P (as in the previous chapter), and they form a set denoted by $\text{Res}(P)$ (on the other hand, when $\theta < 0$, the eigenvalues of P_θ are just the complex conjugates of the resonances of P, and are called anti-resonances).

Let us observe that the resonances of P can also be viewed as the poles of the meromorphic extension, from $\{\text{Im } z > 0\}$, of some matrix elements of the resolvent $R(z) := (P - z)^{-1}$ as in (6) of (1).

It is proved in [HeSj1, HeSj2] that, in this situation, the resonances of P near 0 are close to the eigenvalues of the operator

$$\widetilde{P} := -h^2\Delta + \widetilde{V} \tag{2.2.1}$$

where $\widetilde{V} \in C^\infty(\mathbb{R}^n;\mathbb{R})$ coincides with V in $\{\mathrm{dis}(x,(M)) \geq \delta\}$ ($\delta > 0$ is fixed arbitrarily small), and is such that $\inf_{\{\mathrm{dis}(x,M)\leq\delta\}} \widetilde{V} > 0$. The precise statement is the following one : Let $I(h)$ be a closed interval containing 0, and $a(h) > 0$ such that $a(h) \to 0$ as $h \to 0_+$, and, for all $\varepsilon > 0$ there exists $C_\varepsilon > 0$ satisfying,

$$a(h) \geq \frac{1}{C_\varepsilon} e^{-\varepsilon/h}; \tag{2.2.2}$$

$$\sigma(\widetilde{P}) \cap ((I(h) + [-2a(h), 2a(h)]) \backslash I(h)) = \emptyset, \tag{2.2.3}$$

for all $h > 0$ small enough. Then, there exists a constant $\varepsilon_1 > 0$ and a bijection,

$$\widetilde{\beta} \, : \, \sigma(\widetilde{P}) \cap I(h) \, \to \, \mathrm{Res}(P) \cap \Gamma(h),$$

where we have set,

$$\Gamma(h) := (I(h) + [-a(h), a(h)]) + i[-\varepsilon_1, 0],$$

such that, for any $\varepsilon > 0$, one has,

$$\widetilde{\beta}(\lambda) - \lambda = \mathcal{O}(e^{-(2S_0-\varepsilon)/h}), \tag{2.2.4}$$

uniformly as $h \to 0_+$.

In particular, since the eigenvalues of $\widetilde{P}$ are real, one obtains that, for any $\varepsilon > 0$, the resonances ρ in $\Gamma(h)$ satisfy,

$$\mathrm{Im}\,\rho = \mathcal{O}(e^{-(2S_0-\varepsilon)/h}). \tag{2.2.5}$$

From now on, we consider the particular case where $I(h)$ consists of a unique value $E(h)$, such that,

$$\begin{aligned} & E(h) \in \sigma_{disc}(\widetilde{P}); \\ & E(h) \to 0 \text{ as } h \to 0_+; \\ & \sigma(\widetilde{P}) \cap [E(h) - 2a(h), E(h) + 2a(h)] = \{E(h)\}, \\ & \text{ where } a(h) \text{ satisfies (2.2.2).} \end{aligned} \tag{2.2.6}$$

Remark 2.2.1. *Let us observe that, by Weyl estimates, one knows that the number of eigenvalues of $\widetilde{P}$ inside any small enough fix interval around 0 is $\mathcal{O}(h^{-n})$, and thus, in particular, is not exponentially large as $h \to 0$. As a consequence, and possibly by restricting the set where h takes its values (e.g. by taking h along a sequence tending to 0_+), it is not difficult to construct many such intervals $I(h)$ satisfying (2.2.6) (see also [HeSj1], Section 2, and [HeSj2], Section 9).*

We denote by u_0 the normalised eigenstate of $\widetilde{P}$ associated with $E(h)$, and, applying (2.2.4), we also denote by $\rho = \rho(h)$ the unique resonance of P such that $\rho - E(h) = \mathcal{O}(e^{-(2S_0-\varepsilon)/h})$.

The purpose is to obtain a lower bound on the width $|\mathrm{Im}\,\rho|$, possibly of the same order of magnitude as the upper bound.

2.3 Main Result

Following the ideas of [Ma1], we consider the following additional assumption of non degeneracy. We denote by G the set of all minimal geodesics (relatively to the Lithner-Agmon distance d_V) between U and $\mathcal{M}$ that meet each boundary ∂U and $\partial\mathcal{M}$ at one point only, and we assume,

Assumption [ND] For all $\varepsilon > 0$ and for all neighborhoods W of the set $\bigcup_{\gamma\in G}(\gamma\cap\partial U)$, there exists $C = C(\varepsilon, W) > 0$ such that, for all $h > 0$ small enough, one has,

$$\|u_0\|_{L^2(W)} \geq \frac{1}{C}e^{-\varepsilon/h}.$$

Our main result is,

Theorem 2.3.1. *Suppose Assumptions 1-3, (2.2.6), and Assumption [ND]. Then, for any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ such that, for all $h > 0$ small enough, one has,*

$$|\mathrm{Im}\,\rho(h)| \geq \frac{1}{C(\varepsilon)}e^{-(2S_0+\varepsilon)/h}. \tag{2.3.1}$$

Remark 2.3.2. *In view of (2.2.5), this lower bound is optimal. Indeed, a consequence of (2.2.5) and (2.3.1) is the following identity:*

$$\lim_{h\to 0_+} h\ln|\mathrm{Im}\,\rho| = -2S_0 \tag{2.3.2}$$

Remark 2.3.3. *Assumption [ND] is always satisfied in the one dimensional case. When $n \geq 2$, thanks to standard properties of propagation of the microsupport (defined in Appendix, for the properties see, e.g., [Ma2]), a sufficient condition to have Assumption [ND] is the following geometrical one (see also [Ma1]): For any neighborhood W in $\mathbb{R}^{2n}$ of $\bigcup_{\gamma\in G}(\gamma\cap\partial U)\times\{0\}$, the set $\bigcup_{t\in\mathbb{R}}\exp tH_p(W)$ is a neighborhood of $\Sigma_0 := \{\xi^2 + V(x) = 0\,,\, x\in U\}$. Obviously, a sufficient condition is: For any open set W intersecting Σ_0, $\bigcup_{t\in\mathbb{R}}\exp tH_p(W)$ is a neighborhood of Σ_0.*

2.4 Reduction to an estimate in $\mathcal{M}$

From now on, we denote by u the resonant state of P associated with the resonance ρ, and normalised in such a way that,

$$\|u\|_{L^2(\ddot{O})} = 1, \tag{2.4.1}$$

where $\ddot{O} := \mathbb{R}^n \backslash \mathcal{M}$. Then, it is well known (see, e.g., [HeSj2], Theorem 9.9) that for any bounded set $\mathcal{B} \subset \mathbb{R}^n$, and for any $\varepsilon > 0$, one has,

$$\|e^{d_V(x,U)/h} u\|_{H^1(\mathcal{B})} = \mathcal{O}(e^{\varepsilon/h}). \tag{2.4.2}$$

In particular, if $\mathcal{B} \subset \mathcal{M}$, then for any $\varepsilon > 0$, one has,

$$\|u\|_{H^1(\mathcal{B})} = \mathcal{O}(e^{-(S_0-\varepsilon)/h}). \tag{2.4.3}$$

Then, if we set,

$$\mathcal{T}_1 := \bigcup_{\gamma \in G} (\gamma \cap \partial\mathcal{M})$$

(the set of "points of type 1" in the terminology of [HeSj2]), and if $\mathcal{B}$ stays away from the set,

$$\mathcal{A} := \Pi_x \left(\bigcup_{t \in \mathbb{R}} \exp tH_p \left(\mathcal{T}_1 \times \{0\}\right) \right),$$

(where Π_x stands for the natural projection $(x,\xi) \mapsto x$, and $H_p := (\partial_\xi p, -\partial_x p)$ is the Hamilton field of $p(x,\xi) := \xi^2 + V(x)$), by [HeSj2], Theorem 9.11, we know that for any $s \geq 0$, there exists $\varepsilon_0 > 0$ and a neighborhood $\mathcal{B}'$ of $\mathcal{B}$ such that,

$$\|u\|_{H^s(\mathcal{B}')} = \mathcal{O}(e^{-(S_0+\varepsilon_0)/h}). \tag{2.4.4}$$

On the other hand, performing Stokes formula on any smooth bounded open domain Ω containing the closure of $\ddot{O}$, we see as in [HeSj2], Formula (10.65), that one has,

$$(\mathrm{Im}\ \rho)\|u\|^2_{L^2(\Omega)} = -h^2 \mathrm{Im} \int_{\partial\Omega} \frac{\partial u}{\partial \nu} \overline{u} ds, \tag{2.4.5}$$

where ds is the surface measure on $\partial\Omega$, and ν stands for the outward pointing unit normal to Ω. Using (2.4.3)-(2.4.5), we deduce that, for some $\varepsilon_0' > 0$, one has,

$$\mathrm{Im}\ \rho = -h^2 \mathrm{Im} \int_{\partial\Omega \cap \mathcal{A}'} \frac{\partial u}{\partial \nu} \overline{u} ds + \mathcal{O}(e^{-(2S_0+\varepsilon_0')/h}), \tag{2.4.6}$$

where $\mathcal{A}'$ is an arbitrarily small neighborhood of $\mathcal{A}$ (indeed, one has $\|u\|_{L^2(\Omega)} = 1 + \mathcal{O}(e^{-\delta/h})$ by (2.4.1)-(2.4.3), and, away from $\mathcal{A}'$, the quantity $e^{2S_0/h} \frac{\partial u}{\partial \nu} \overline{u}$ is exponentially small in virtue of (2.4.4), while on $\mathcal{A}'$ it is $\mathcal{O}(e^{\varepsilon/h})$ for all $\varepsilon > 0$).

In order to transform this expression into a more practical one, we plan to use the analytic pseudofifferential calculus introduced in [Sj]. For this purpose, we first have to prove some a priori estimate on u near $\mathcal{A}$.

So, let $z_1 \in \mathcal{T}_1$, let W_1 be a neighborhood of z_1 in $\partial\mathcal{M}$, and for $t_0 > 0$ sufficiently small, consider the two Lagrangian manifolds,

$$\Lambda_\pm := \bigcup_{0<\pm t<2t_0} \exp tH_p(W_1 \times \{0\}) \quad (\subset \{p = 0\}).$$

(Note that they are Lagrangian because $W_1 \times \{0\}$ is isotropic.) Then, it is easy to check that $\Lambda_\pm$ projects bijectively on the base, and since $p(x,\xi)$ is an even function of ξ, we see that they can be represented by an equation of the type,

$$\Lambda_\pm \,:\, \xi = \pm\nabla\psi(x),$$

where ψ is a real-analytic function, such that,

$$(\nabla\psi(x))^2 + V(x) = 0. \tag{2.4.7}$$

Now, we set $z_0 := \Pi_x\left(\exp t_0H_p(z_1,0)\right)$, and we still denote by ψ an holomorphic extension of ψ to a complex neighborhood of z_0. We have,

Proposition 2.4.1. *For any $\varepsilon_1 > 0$, one has,*

$$e^{-i\psi/h}u \in H_{-S_0+\varepsilon_1|\mathrm{Im}\, x|,z_0},$$

where $H_{-S_0+\varepsilon_1|\mathrm{Im}\, x|,z_0}$ is the Sjöstrand's space consisting of h-dependent holomorphic functions $v = v(x;h)$ defined near z_0, such that, for all $\varepsilon > 0$,

$$v(x,h) = \mathcal{O}(e^{(-S_0+\varepsilon_1|\mathrm{Im}\, x|+\varepsilon)/h}),$$

uniformly for x close to z_0 and $h > 0$ small enough.

Proof. Set

$$v(x,h) := e^{-i\psi/h+S_0/h}u(x,h). \tag{2.4.8}$$

We have to prove that $v \in H_{\varepsilon_1|Imx|,z_0}$ for all $\varepsilon_1 > 0$.

Let $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^n)$ supported in a small neighborhood of z_0, and such that $\chi = 1$ near z_0. Setting $\varphi(x,y,\tau) := (x-y)\tau + \frac{1}{2}i(x-y)^2$ and $a(x,\tau) := 1 + \frac{1}{2}ix\tau$, for $x \in \{\chi = 1\}$ we can write (see, e.g., formula (6.9) in [Sj]),

$$v(x) = (2\pi)^{-n}\int e^{i|\xi|\varphi(x,y,\frac{\xi}{|\xi|})}a(x-y,\frac{\xi}{|\xi|})v(y)\chi(y)dyd\xi, \tag{2.4.9}$$

Moreover, by (2.4.3) we already know that, on the real axis, v cannot be exponentially large, that is, for any $\varepsilon > 0$, one has,

$$v = \mathcal{O}(e^{\varepsilon/h}) \text{ locally uniformly on } \mathbb{R}^n.$$

In addition, v is solution to

$$((hD_x + \nabla\psi)^2 + V - \rho)v = 0. \tag{2.4.10}$$

We set,

$$Q(y, hD_y) := (hD_y + \nabla\psi)^2 + V(y) - \rho,$$

and, in order to estimate the integral, as in [Ma1], we first plan to construct a symbol $b = b(x, y, \tau, \xi, h) \sim \sum_{k\geq 0} b_k(x, y, \tau, h)|\xi|^{-k}$, with large parameter $|\xi|$, in such a way that one has,

$$e^{-i|\xi|\varphi(x,y,\tau)t}Q(y, hD_y)\left(e^{i|\xi|\psi(x,y,\tau)}b\right) \sim a(x - y, \tau). \tag{2.4.11}$$

Here, the asymptotic must hold as $|\xi| \to \infty$, and the quantities $\tau \in S^{n-1}$, $\mu := \frac{1}{h|\xi|} \in (0, \frac{1}{C}]$ (with $C > 0$ large enough) have to be considered as extra parameters. In particular, (2.4.11) can be rewritten as,

$$\left[(-D_y + \mu|\xi|\nabla\psi(y) - |\xi|\nabla_y\varphi)^2 + \mu^2|\xi|^2(V - \rho)\right] b \sim a(x - y, \tau)\mu^2|\xi|^2. \tag{2.4.12}$$

Since $(\nabla\psi)^2 = E_0 - V$ and $\rho \to E_0$ as $h \to 0_+$, the (leading order) coefficient c_2 of $|\xi|^2$ satisfies,

$$\begin{aligned} c_2 &= (\mu\nabla\psi - \nabla_y\varphi)^2 + \mu^2(V - \rho) \\ &= (\nabla_y\varphi)^2 - 2\mu\nabla_y\varphi\nabla\psi + o(1) \\ &= (-\tau - i(x - y))^2 + 2\mu(\tau - i(x - y))\nabla\psi + o(1) \\ &= 1 + \mathcal{O}(|x - y| + \mu) + o(1). \end{aligned}$$

In particular, we can solve the transport equations for x, y close enough to z_0, and for μ small enough, that is, $|\xi| \geq C/h$ with $C > 0$ sufficiently large. By the microlocal analytic theory of [Sj], we also know that the resulting formal symbol admits analytic estimates, and can therefore be re-summed into a symbol $b(x, y, \tau, \xi, h)$ such that, for some constant $\delta > 0$, one has,

$$e^{-i|\xi|\varphi(x,y,\tau)t}Q(y, hD_y)\left(e^{i|\xi|\psi(x,y,\tau)}b\right) - a(x - y, \tau) = \mathcal{O}(e^{-\delta|\xi|}), \tag{2.4.13}$$

uniformly with respect to $\tau \in S^{n-1}$, $|\xi| \geq C/h$, $h > 0$ small enough, and $x, y \in \mathbb{C}^n$ close enough to z_0.

Then, splitting the integral in (2.4.9), we write,

$$v(x) = \int_{\{|\xi|\geq \frac{C}{h}\}} + \int_{\{|\xi|\leq \frac{\varepsilon_1}{h}\}} + \int_{\{\frac{\varepsilon_1}{h}\leq|\xi|\leq \frac{C}{h}\}} . \qquad (2.4.14)$$

The first integral can be estimated by using (2.4.13), an integration by part, and the fact that v solves $Qv = 0$. One finds that it is $\mathcal{O}(e^{-\delta_1/h})$ for some $\delta_1 > 0$.

The second integral can be estimated as in [Ma1], and it is $\mathcal{O}(e^{\varepsilon_1|Imx|/h})$.

For the third integral, we make the change of variable $\xi = \eta/h$, and we find,

$$h^{-n}\int_{\{\varepsilon_1\leq|\eta|\leq C\}} e^{i(x-y)\eta/h-|\eta|(x-y)^2/2h} a(x-y, \frac{\eta}{|\eta|})\chi(y)v(y)dyd\eta. \qquad (2.4.15)$$

But, from the theory of [HeSj2], we know that if u is outgoing, then, near z_0, the microsupport of u satisfies,

$$MS(ue^{S_0/h}) \subset \Lambda_+.$$

Since $\Lambda_+ = \{\nabla\psi(y); y \text{ close to } z_0\}$, by standard rules on the microsupport we deduce,

$$MS(v) \subset \{\eta = 0\}.$$

As a consequence, the integral appearing in (2.4.15) is $\mathcal{O}(e^{-\delta_2/h})$ for some $\delta_2 > 0$, and the result follows. □

Thanks to this proposition, we can enter the framework of the analytic pseudodifferential calculus of [Sj]. We set $v := e^{-i\psi/h}u$, and, in a complex neighborhood of z_0, we can write $Pu = e^{-i\psi/h}Pe^{i\psi/h}v$ as (see [Sj], Section 4, in particular Remark 4.4),

$$Pu(x) = \frac{1}{(2\pi h)^n}\int_{\Gamma(x)} e^{i(x-y)\alpha_\xi/h-[(x-\alpha_x)^2+(y-\alpha_x)^2]/2h} p_\psi(\alpha_x, \alpha_\xi)v(y)dyd\alpha, \quad (2.4.16)$$

where p_ψ is the symbol of $P_\psi := e^{-i\psi/h}Pe^{i\psi/h}$, and satisfies,

$$p_\psi(\alpha) = (\alpha_\xi + \nabla\psi(\alpha_x))^2 + V(\alpha_x) + \mathcal{O}(h), \qquad (2.4.17)$$

and where $\Gamma(x)$ is the (singular) complex contour of integration given by,

$$\Gamma(x)\ :\ \begin{cases} \alpha_\xi = 2i\varepsilon_1\dfrac{\overline{x-y}}{|x-y|}\ ; \\ |x-y| \leq r,\ y\in\mathbb{C}^n\ (r \text{ small enough with respect to } \varepsilon_1)\,; \\ |x-\alpha_x| \leq r,\ \alpha_x\in\mathbb{R}^n. \end{cases}$$

Let us observe that the identity (2.4.16) takes place in $H_{-S_0+\varepsilon_1|\mathrm{Im}\, x|,z_0}$, that is, modulo error terms that are exponentially smaller than $e^{(-S_0+\varepsilon_1|\mathrm{Im}\, x|)/h}$ in a complex neighborhood of z_0.

Taking local coordinates $(x', x_n) \in \mathbb{R}^{n-1}\times\mathbb{R}$ near z_1, in such a way that $dV(z_1)\cdot x = -cx_n$ with $c > 0$ (and thus $T_{z_1}\partial\mathcal{M} = \{x_n = 0\}$), we see that $\nabla\psi(x)$ remains close to $(0, \sqrt{x_n})$. In particular, still working in these coordinates, the symbol $\rho - V(x) - (\xi' + \nabla_{x'}\psi(x))^2$ is elliptic along $\Gamma(x)$ (at least if ε_1 has been chosen sufficiently small), and with positive real part. Thus, in view of (2.4.17), so is $(\xi_n + \partial_{x_n}\psi(x))^2 - p_\psi(x,\xi) + \rho$. As a consequence, applying the symbolic calculus of [Sj], we conclude to the existence of a pseudodifferential operator $A = A(x, hD_{x'})$, with principal symbol,

$$a(x,\xi') = \sqrt{\rho - V(x) - (\xi' + \nabla_{x'}\psi(x))^2},$$

such that $P_\psi - \rho$ can be factorised as,

$$P_\psi - \rho = (hD_{x_n} + \partial_{x_n}\psi(x) + A)\circ(hD_{x_n} + \partial_{x_n}\psi(x) - A),$$

when acting on $H_{-S_0+\varepsilon_1|\mathrm{Im}\, x|,z_0}$. Since $(P_\psi - \rho)v = 0$, and $hD_{x_n} + \partial_{x_n}\psi(x) + A$ is elliptic along $\Gamma(x)$, we deduce,

$$(hD_{x_n} + \partial_{x_n}\psi(x) - A)v = 0 \quad \text{in } H_{-S_0+\varepsilon_1|\mathrm{Im}\, x|,z_0}. \tag{2.4.18}$$

Now, going back to (2.4.6), and choosing Ω in such a way that its boundary contains z_0 and is of the form $\{x_n = \delta_0\}$ (with $\delta_0 > 0$ constant) near z_0, the corresponding part of the integral can be written as,

$$I_0 := -h^2\mathrm{Im}\int_{\{x_n=\delta_0\}\cap W_0}\left(\frac{\partial v}{\partial x_n} + \frac{i}{h}\frac{\partial\psi}{\partial x_n}v\right)\overline{v}dx'$$

where W_0 is a small real neighborhood of z_0. Thus, using (2.4.18), we obtain,

$$I_0 = -h\mathrm{Re}\int_{\{x_n=\delta_0\}\cap W_0}(Av)\overline{v}dx' + \mathcal{O}(e^{-(2S_0+\varepsilon_0)/h}),$$

with $\varepsilon_0 > 0$. Finally, observing that the principal symbol of A is strictly positive in $(z_0, 0)$, and proceeding as in [Ma1], Section 2 (in particular, considering the realisation on the real of A), we can construct an elliptic pseudodifferential operator B of order 0, such that,

$$A = B^*B + \mathcal{O}(e^{-(S_0+\varepsilon)/h})$$

on $L^2(\{x_n = 0\}\cap W_0)$ (with some $\varepsilon > 0$). Finally, taking advantage of the ellipticity of B, we conclude, as in [Ma1], Lemma 2.3, that we have,

$$I_0 \le -\frac{h}{C}\|v\|^2_{L^2(\{x_n=0\}\cap W_0)} + \mathcal{O}(e^{-(2S_0+\varepsilon_0)/h}),$$

where C, ε_0 are positive constants. Summing up all the contributions, and observing that, in the previous formula, v may be replaced by u (since ψ is real on the real and $v = e^{-i\psi/h}u$), we have proved,

Proposition 2.4.2. *There exist $C, \varepsilon_0 > 0$ such that,*

$$|\mathrm{Im}\ \rho| \geq \frac{h}{C}\|u\|^2_{L^2(\partial\Omega)} - Ce^{-(2S_0+\varepsilon_0)/h},$$

uniformly for $h > 0$ small enough.

From now on, we proceed by contradiction : We assume the existence of $\varepsilon_1 > 0$ such that,

$$|\mathrm{Im}\ \rho| = \mathcal{O}(e^{-2(S_0+\varepsilon_1)/h}), \tag{2.4.19}$$

uniformly as $h \to 0_+$ (possibly along a sequence of numbers only). By the previous proposition, this implies,

$$\|u\|_{L^2(\partial\Omega)} = \mathcal{O}(e^{-(S_0+\varepsilon_1)/h}). \tag{2.4.20}$$

2.5 Propagation across $\partial\mathcal{M}$

The purpose of this section is to propagate the estimate (2.6.1) up to the boundary of $\mathcal{M}$ and beyond. From now on, we specify the choice of Ω by taking,

$$\Omega := \ddot{O} \cup \{V(x) > -\delta_0\},$$

where $\delta_0 > 0$ will be fixed small enough later on (in particular, one has $V = -\delta_0$ on $\partial\Omega$).

In order to propagate (2.6.1) across $\partial\mathcal{M}$, we use explicit Carleman estimates, in a spirit similar to that of [DGM] (see also [KSU]).

We denote by $\mathcal{N}$ some fix neighborhood of $\partial\mathcal{M}$, and, for δ_0 small enough and $\delta \in (0, \delta_0)$, we consider the neighborhood of $\partial\mathcal{M}$ given by,

$$Z_\delta := \{x \in \mathcal{N}\,;\, -\delta_0 \leq V(x) \leq \delta\},$$

We also set,

$$\Sigma_\delta := \{x \in \mathcal{N}\,;\, V(x) = \delta\};$$
$$\Sigma_0 := \{x \in \mathcal{N}\,;\, V(x) = -\delta_0\},$$

so that we have,

$$\partial\Omega = \Sigma_0 \quad ; \quad \partial Z_\delta = \Sigma_\delta \cup \Sigma_0.$$

By (2.6.1), we have,

$$\|u\|_{L^2(\Sigma_0)} = \mathcal{O}(e^{-(S_0+\varepsilon_0)/h}), \tag{2.5.1}$$

for some constant $\varepsilon_0 > 0$, and, using the equation $Pu = \rho u$ and the (standard) ellipticity of P, we obtain similar estimates on the derivatives of u, too.

As in [Ma1], Section 2 (in particular the proof of Lemma 2.1), one can see that inside $\partial\mathcal{N} \cap \{V > 0\}$, the Lithner-Agmon distance to $\partial\mathcal{M}$ is given by,

$$d_V(x, \mathcal{M}) = G(x, \sqrt{V(x)}), \tag{2.5.2}$$

where G is an analytic function, and $G(x, s) \sim s^3$ as $s \to 0_+$. Actually, this result is obtained by using a technique taken from [HeSj2], and consisting in representing the Lagrangian Λ_0 generated by the nul-bicharacteristics of $q(x, \xi) := \xi^2 - V(x)$ merging from $\partial\mathcal{M} \times \{0\}$ locally as,

$$\Lambda_0 \quad : \quad \begin{cases} -x_n = \frac{\partial g}{\partial \xi_n}(x', \xi_n) \\ \xi' = \nabla_{x'} g(x', x_n), \end{cases}$$

where the local Euclidean coordinates (x', x_n) (centered at some arbitrary point of $\mathcal{M}$) have been chosen in such a way that $V(x) = -C_0 x_n + \mathcal{O}(|x|^2)$ near that point, and where g is analytic near 0 and satisfies $g(0) = 0$, $\nabla g(0) = 0$. Then, using that the projection $\Lambda_0 \ni (x, \xi) \mapsto x$ is bijective above $\{V > 0\}$, one can see in a way similar to that in [HeSj2], Section 10 (in particular Formula (10.15)) that on this set one has,

$$d(x, \partial\mathcal{M}) = -\text{c.v.}_{\xi_n}(x_n \xi_n + g(x', \xi_n)),$$

where the notation c.v._{ξ_n} stands for the critical value with respect to the variable ξ_n, and where the critical point is chosen in such a way that $d(x, \partial\mathcal{M})$ is a decreasing function of x_n. Finally, using that g is a solution to the eikonal equation,

$$(\nabla_{x'} g)^2 + \xi_n^2 = V(x', -\partial_{x_n} g),$$

(2.5.2) follows by taking a second order Taylor expansion of g with respect to ξ_n at $\xi_n = 0$ (observe that, in contrast with the situation in [HeSj2], in our case the caustic set corresponds to the singularities of the distance to $\partial\mathcal{M}$, and thus is exactly $\partial\mathcal{M}$; as a consequence, one has the equivalence $\partial^2_{\xi_n} g = 0 \Leftrightarrow \xi_n = 0$, together with the property $\nabla_{x'} g(x', 0) = 0$).

Now, by the triangle inequality, we have,

$$d_V(U, x) \geq S_0 - d_V(x, \mathcal{M}),$$

and thus, by (2.5.2), we deduce the existence of a constant $c_0 > 0$ such that,

$$d_V(U, x) \geq S_0 - c_0 \max(V(x), 0)^{3/2}$$

in all of Z_δ. As a consequence, by (2.4.2), for any $\delta, \varepsilon > 0$ small enough, one has,

$$u = \mathcal{O}(e^{-(S_0 - c_0\delta^{3/2} - \varepsilon)/h}) \text{ on } Z_\delta, \tag{2.5.3}$$

and similarly for all the derivatives of u.

Proposition 2.5.1. *For $\delta > 0$ sufficiently small, there exists $\varepsilon_\delta > 0$ such that,*

$$\|u\|_{L^2(Z_\delta)} = \mathcal{O}(e^{-(S_0+\varepsilon_\delta)/h}),$$

uniformly for $h > 0$ small enough.

Proof. The proof relies on some explicit Carleman-type estimates, in a way rather similar to that of [DGM]. We set,

$$v := e^{\alpha(\delta - V(x))/h} u,$$

where $\alpha > 0$ is fixed sufficiently small in order to have

$$2\alpha\delta_0 < \varepsilon_0/2, \tag{2.5.4}$$

where ε_0 is that of (2.5.1). The function v is solution to,

$$(-h^2\Delta + V - \rho - \alpha^2(\nabla V)^2 - 2h\alpha(\nabla V)\cdot\nabla - h\alpha(\Delta V))v = 0,$$

that is,

$$(A + iB)v = 0,$$

where A and B are the two formally selfadjoint operators given by,

$$A := -h^2\Delta + V - \text{Re}\,\rho - \alpha^2(\nabla V)^2 \quad ; \quad B := -2h\alpha(\nabla V)\cdot D_x - \text{Im}\,\rho + ih\alpha(\Delta V).$$

In addition, by (2.5.3), for any $\varepsilon > 0$, we also have,

$$\|v\|_{H^2(\Sigma_\delta)} = \mathcal{O}(e^{-(S_0 - c_0\delta^{3/2} - \varepsilon)/h}), \tag{2.5.5}$$

and, by (2.5.4),

$$\|v\|_{H^2(\Sigma_0)} = \mathcal{O}(e^{-(S_0+\varepsilon_1)/h}), \tag{2.5.6}$$

where $\varepsilon_1 := \varepsilon_0/2$. Then, we write,

$$0 = \|(A+iB)v\|^2_{L^2(Z_\delta)} = \|Av\|^2_{L^2(Z_\delta)} + \|Bv\|^2_{L^2(Z_\delta)} + 2\text{Im}\,\langle Av, Bv\rangle_{L^2(Z_\delta)}, \tag{2.5.7}$$

and the key-point is the following Carleman estimate:

Lemma 2.5.2. *If α and δ_0 has been chosen sufficiently small, then, there exists a constant $C>0$ such that, for all $\delta>0$ small enough, one has,*

$$\text{Im } \langle Av,Bv\rangle_{L^2(Z_\delta)} \geq \frac{h}{C}\|v\|^2_{L^2(Z_\delta)} - Ch\|Av\|^2_{L^2(Z_\delta)} - C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}. \quad (2.5.8)$$

Proof. Using Green's formula, together with (2.5.5)-(2.5.6) and the fact that A and B are formally selfadjoint, we immediately obtain,

$$\text{Im } \langle Av,Bv\rangle_{L^2(Z_\delta)} = \frac{i}{2}\langle [A,B]v,v\rangle_{L^2(Z_\delta)} + \mathcal{O}(e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}),$$

where $\varepsilon>0$ is arbitrarily small. Then, we compute,

$$[A,B] = \alpha[-h^2\Delta, -2h(\nabla V)\cdot D_x + ih(\Delta V)] - 2h\alpha[V-\alpha^2(\nabla V)^2, (\nabla V)\cdot D_x].$$

By setting $Q_2 := 2\sum_{j,k}(\partial_j\partial_k V)\partial_j\partial_k$, $Q_1 := \nabla(\Delta V)\cdot\nabla$ and $Q_0 := (\nabla V)\cdot(\nabla(\Delta V)^2)$ (of order 2, 1, and 0, respectively), we find,

$$[A,B] = -2i\alpha h^3(Q_2+Q_1) - i\alpha h^3((\Delta^2 V)+2Q_1) - 2i\alpha h(\nabla V)^2 + 2i\alpha^3 hQ_0, \quad (2.5.9)$$

that is,

$$\frac{i}{2}[A,B] = \alpha h^3(Q_2+2Q_1+\frac{1}{2}(\Delta^2 V)) + \alpha h(\nabla V)^2 - \alpha^3 hQ_0.$$

Now, our assumptions imply that ∇V does not vanish on $\partial\mathcal{M}$ and thus also on Z_δ if δ_0 has been chosen sufficiently small and $\delta\in(0,\delta_0]$. Therefore, there exists a constant $C_0>0$ (independent of δ,δ_0 small enough) such that,

$$\langle(\nabla V)^2 v,v\rangle_{L^2(Z_\delta)} \geq \frac{1}{C_0}\|v\|^2_{L^2(Z_\delta)}.$$

Using (2.5.9), we deduce,

$$\begin{aligned}\text{Im } \langle Av,Bv\rangle_{L^2(Z_\delta)} \geq & \frac{h\alpha}{C_0}\|v\|^2_{L^2(Z_\delta)} + \alpha h^3 \text{Re } \langle Q_2 v,v\rangle_{L^2(Z_\delta)} \\ & + 2\alpha h^3 \text{Re } \langle Q_1 v,v\rangle_{L^2(Z_\delta)} - C_1(\alpha h^3+\alpha^3 h)\|v\|^2_{L^2(Z_\delta)} \\ & - C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h},\end{aligned} \quad (2.5.10)$$

where $C_1, C_\varepsilon>0$ are constants that do not depend on h and α (and actually nor on δ,δ_0).

Since Q_1 is a real vector-field, by Green's formula and (2.5.5)-(2.5.6) we easily obtain,

$$\text{Re } \langle Q_1 v,v\rangle_{L^2(Z_\delta)} = \mathcal{O}(\|v\|^2_{L^2(Z_\delta)} + e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}). \quad (2.5.11)$$

Moreover, still by Green's formula and (2.5.5)-(2.5.6), we have,

$$\begin{aligned} h^2\text{Re}\,\langle Q_2 v, v\rangle_{L^2(Z_\delta)} & \\ &= \mathcal{O}(h^2\|\nabla v\|^2_{L^2(Z_\delta)} + h^2\|v\|^2_{L^2(Z_\delta)} + e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}) \\ &= \mathcal{O}(|\langle h^2\Delta v, v\rangle_{L^2(Z_\delta)}| + h^2\|v\|^2_{L^2(Z_\delta)} + e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}), \end{aligned}$$

and thus, for any constant $C>0$ arbitrarily large,

$$\begin{aligned} h^2|\text{Re}\,\langle Q_2 v, v\rangle_{L^2(Z_\delta)}| & \\ &\leq C\|h^2\Delta v\|^2_{L^2(Z_\delta)} + \frac{1}{C}\|v\|^2_{L^2(Z_\delta)} + C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}. \end{aligned} \tag{2.5.12}$$

Since we also have,

$$\|h^2\Delta v\|_{L^2(Z_\delta)} \leq \|Av\|_{L^2(Z_\delta)} + \|(V - \text{Re}\,\rho - \alpha^2(\nabla V)^2)v\|_{L^2(Z_\delta)},$$

and $|V - \text{Re}\,\rho - \alpha^2(\nabla V)^2| \leq 2\delta_0 + C_2\alpha^2$ (where $C_2 := \sup_{\ddot{O}}|\nabla V|^2$) on Z_δ, we deduce from (2.5.12) that, for any $C>0$, one has,

$$\begin{aligned} h^2|\text{Re}\,\langle Q_2 v, v\rangle_{L^2(Z_\delta)}| & \\ \leq C\|Av\|^2_{L^2(Z_\delta)} &+ (\frac{1}{C} + 2C\delta_0 + CC_2\alpha^2)\|v\|^2_{L^2(Z_\delta)} + C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}. \end{aligned}$$

Choosing first C sufficiently large, then δ_0 and α sufficiently small, in such a way that

$$\frac{1}{C} + 2C\delta_0 + CC_2\alpha^2 \leq \frac{1}{2C_0},$$

this gives,

$$\begin{aligned} h^2|\text{Re}\,\langle Q_2 v, v\rangle_{L^2(Z_\delta)}| & \\ \leq C\|Av\|^2_{L^2(Z_\delta)} &+ \frac{1}{2C_0}\|v\|^2_{L^2(Z_\delta)} + C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}. \end{aligned} \tag{2.5.13}$$

Inserting (2.5.11) and (2.5.13) into (2.5.14), we finally obtain,

$$\begin{aligned} \text{Im}\,\langle Av, Bv\rangle_{L^2(Z_\delta)} \geq & \frac{h\alpha}{2C_0}\|v\|^2_{L^2(Z_\delta)} - 2C\alpha h\|Av\|^2_{L^2(Z_\delta)} \\ & - C_1'(\alpha h^3 + \alpha^3 h)\|v\|^2_{L^2(Z_\delta)} - C_\varepsilon e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}, \end{aligned} \tag{2.5.14}$$

where C_1' is some new constant, and the result follows by shrinking α again. □

Inserting (2.5.8) into (2.5.7), for h small enough we obtain,

$$\|v\|^2_{L^2(Z_\delta)} = \mathcal{O}(e^{-2(S_0-c_0\delta^{3/2}-\varepsilon)/h}),$$

and therefore, since $2\alpha(\delta - V) \geq \alpha\delta$ on $Z_{\delta/2} \subset Z_\delta$,

$$\|u\|^2_{L^2(Z_{\delta/2})} = \mathcal{O}(e^{-(2S_0+\alpha\delta-2c_0\delta^{3/2}-2\varepsilon)/h}).$$

Observing that α has been chosen independently of δ, we obtain the result of Proposition 2.5.1 by taking δ sufficiently small in order to have $\alpha\delta > 2c_0\delta^{3/2}$. □

2.6 Completion of the proof

We recall that we have proceeding by contradiction, assuming condition (2.4.19) at the end of section (2.4), that implies the estimate (2.6.1),

$$\|u\|_{L^2(\partial\Omega)} = \mathcal{O}(e^{-(S_0+\varepsilon_1)/h}), \tag{2.6.1}$$

thanks to the proposition (2.4.2).

From this point, the proof proceeds exactly as in [Ma1]. More precisely, if $\widetilde{P} = -h^2\Delta + \widetilde{V}$ is the operator defined as in (2.2.1), with $\widetilde{V} = V$ near $\ddot{O}\backslash Z_{\delta/2}$, we already know (see [HeSj2], Theorem 9.9) that the difference $u - u_0$ satisfies,

$$\|e^{d_V(U,x)/h}(u-u_0)\|_{L^2(\ddot{O}\backslash Z_{\delta/2})} = \mathcal{O}(e^{-\varepsilon_3/h}),$$

for some constant $\varepsilon_3 = \varepsilon_3(\delta) > 0$. Then, applying Proposition 2.5.1, we deduce,

$$\|e^{d_V(U,x)/h}u_0\|_{L^2(Z_\delta\backslash Z_{\delta/2})} = \mathcal{O}(e^{-\varepsilon_4/h}),$$

with $\varepsilon_4 = \varepsilon_4(\delta) > 0$. At this point, we are in a situation absolutely similar to that of [Ma1]. In particular, the previous estimate can be propagated up to the well U along any minimal geodesic $\gamma \in G$, and as in [Ma1], Section 6, we obtain that for all $x_1 \in \bigcup_{\gamma\in G}(\gamma \cap \partial U)$, one has,

$$(x_1, 0) \notin MS(u_0),$$

where $MS(u)$ stands for the microsupport of u as defined by formula (16) in (3.5) and e.g., in [Ma2] (it was called $FS_a(u)$ in [Ma1]). In fact, as in [Ma1], section 3, we can construct a function $F_\pm(y,z)$, and a symbol $a_\pm = a_\pm(y,z;h)$, such that

$$v_\pm := a_\pm(y,z,h)e^{-F_\pm(y,z)/h} \tag{2.6.2}$$

are asymptotic solutions of the equation

$$(P(z,hD_z) - E)\, v_\pm(y,z,h) = 0, \tag{2.6.3}$$

where $y \in \gamma \cap \{V(x) > 0\}$ and $z \in \gamma \cap \{V(x) \leq 0\}$.

Choosing local coordinates, we denote by Γ the hypersurface that cut transversally the projection α_y of the outgoing bicharacteristic of $p = \xi^2 + V(x)$, and by Σ the hypersurface that cut $\gamma \in G$ transversally in $y_0 \in \{V(x) > 0\}$.

There exists then $w(y) = \alpha_y \cup \Gamma$ such that $F_\pm(y, w(y)) = 0$ and

$$Re\,(F_\pm) \geq \frac{1}{c}|z - w(y)|^2, \tag{2.6.4}$$

for $z \in \Gamma$ and $y \in \Sigma$; and if y' and z' are local coordinates on Σ and Γ respectively, one can see that

$$det \nabla_{y'} \nabla_{z'} Re\,(F_{\pm}(y_0, w(y_0))) \neq 0.$$

Thanks to these properties, the application $H^{loc}_{C_0|\mathrm{Im}\, z'|}(\Gamma) \ni w \mapsto \int_\Gamma w v_\pm dz'$ is a FBI-transform as defined in (16), and permits us to characterize the microsupport $MS(w)$.

Furthermore, $\nabla_{z'} Re\,(F_\pm(y, w(y))) = 0$, and we can apply to the computation in (2.4) the same consideration of [Ma1], Prop. (4.2): Since $\|u_0\|_{L^2(\Sigma)} = \mathcal{O}(e^{-(S_0+\varepsilon_0)/h})$, there exists $\varepsilon_5 > 0$ such that

$$\int_\Gamma (\frac{\partial u}{\partial x_n} \pm {}^t A u) v_\pm dx' = \mathcal{O}(e^{-\varepsilon_5/h}), \tag{2.6.5}$$

where A is an elliptic pseudodifferential operator.

Thus $(x_1', 0) \notin MS\left((\frac{\partial u_0}{\partial x_n} \pm {}^t A u_0)|_\Gamma\right)$, and that means that $(x_1', 0) \notin MS\left((\frac{\partial u_0}{\partial x_n}|_\Gamma\right) \cup MS\left({}^t A u_0)|_\Gamma\right)$. Taking into account the ellipticity of the symbol of A, we know by composition of pseudodifferential operators, that $(x_1', 0) \notin MS(u_0|_\Gamma)$. By proposition (4.5.1.) in [Ma2], and standard propagation of the microsupport, one can deduce,

$$(x_1, 0) \notin MS(u_0).$$

Then, applying theorem (4.2.2.) of [Ma2], one has $MS(u_0) \subset p^{-1}(0)$, and since

$$(\partial U \times \mathbb{R}^n) \cap p^{-1}(0) \subset \{\xi = 0\},$$

we deduce

$$MS(u_0) \cap \left(\bigcup_{\gamma \in G} (\gamma \cap \partial U) \times \mathbb{R}^n \right) = \emptyset,$$

and thus by standard properties of $MS(u)$ (see, e.g., [Ma2]), we conclude as in [Ma1], Prop. (5.2), the existence of a neighborhood W of $\bigcup_{\gamma \in G}(\gamma \cap \partial U)$ and of a positive constant $\varepsilon_7 > 0$, such that,

$$\|u_0\|_{L^2(W)} = \mathcal{O}(e^{-\varepsilon_7/h}),$$

uniformly for $h > 0$ small enough. But this is in contradiction with Assumption [ND], and the proof of Theorem 2.3.1 is complete.

Chapter 3

Resonances near a Singularity in One Dimension

3.1 Notations and Assumptions

We consider now the semiclassical Schrödinger operator $P = -h^2\partial_x^2 + V$ on $\mathbb{R}$, and we investigate some spectral properties near some fixed energy level $\lambda \in \mathbb{C}$, in order to find resonances, where the potential V is a smooth real-valued function, with a singularity at the origin that leads to a particular wedge shape.
We compute the solutions for the Schrödinger equation

$$(P - \lambda)u = 0, \qquad \mathrm{Im}\,\lambda > 0, \tag{3.1.1}$$

in order to describe the behavior of the resonances. In section (3.2) we compute a simplified linear potential $V : \mathbb{R} \to \mathbb{R}, V = -|x|$, where its symmetry permits us to find an expression directly involving the zeros of Airy functions and their derivatives (some basic formulas for these functions are in the appendix). In section (3.3) we generalize the computation by slightly relax the shape of the potential in two steps, varying the slopes by multiplication with different coefficients. The solutions of the equation coming from computing the transmission coefficient turn out to be more difficult to express in terms of the Airy functions. In section (3.4) we state a general theorem for the existence of a set of resonances, using formulas that still involve Airy functions and their derivatives. In order to find resonances one constructs the meromorphic continuation of the resolvent kernel in the lower complex half-plane; its singularities represent the resonance of the Schrödinger operator, thus the quantization condition leads to nullify the Wronskian computed on the extension of the solutions.

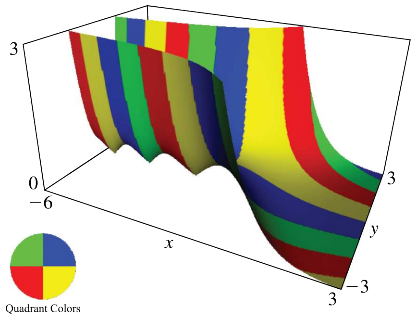


Figure 3.1: $\|Ai(x+iy)\|$

3.2 Tunneling by a linear wedge barrier

From now on P will denote its self-adjoint realization.

Definition 7. Let $x \in \mathbb{R}, \lambda \in \mathbb{C},\ 0 < \text{Im}\ \lambda << 1$. Set $\omega = e^{i\frac{2}{3}\pi}$ as in Appendix (3.6).

$$\begin{aligned} u_+(x,\lambda) &:= Ai(-\frac{\omega}{h^{2/3}}(x+\lambda)), \\ u_-(x,\lambda) &:= Ai(\frac{\omega}{h^{2/3}}(x-\lambda)). \end{aligned} \tag{3.2.1}$$

Proposition 3.2.1.

$$u_+(x,\lambda) \quad \textit{solves } (-h^2\partial_x^2 - x - \lambda)u_+(x,\lambda) = 0 \quad \textit{for } x \geq 0; \tag{3.2.2}$$

Proof. By natural computation, applying the Airy equation we obtain:

$$\begin{aligned} \partial_x u_+(x,\lambda) &= -\frac{\omega}{h^{2/3}} Ai'\left(-\frac{\omega}{h^{2/3}}(x+\lambda)\right) \\ \partial_x^2 u_+(x,\lambda) &= \frac{\omega^2}{h^{4/3}} Ai''\left(-\frac{\omega}{h^{2/3}}(x+\lambda)\right) = \\ \frac{\omega^2}{h^{4/3}}\left(-\frac{\omega}{h^{2/3}}(x+\lambda)\right) & Ai\left(-\frac{\omega}{h^{2/3}}(x+\lambda)\right) = \\ -\frac{\omega^3}{h^2}(x+\lambda) & Ai\left(-\frac{\omega}{h^{2/3}}(x+\lambda)\right) = \\ & -\frac{(x+\lambda)}{h^2}u_+(x,\lambda). \end{aligned} \tag{3.2.3}$$

□

A similar computation shows the same property for u_- :

Proposition 3.2.2.

$$u_-(x,\lambda) \ \textit{solves } (-h^2\partial_x^2 + x - \lambda)u_-(x,\lambda) = 0 \quad \textit{for } x < 0. \tag{3.2.4}$$

Remark 3.2.3. The oscillatory behavior at $\pm\infty$ of the Airy functions permits us to consider u_-, u_+ as acting in the following way:

$$\begin{aligned} u_+(x,\lambda) &= o(1) \quad x \to +\infty; \\ u_-(x,\lambda) &= o(1) \quad x \to -\infty. \end{aligned} \tag{3.2.5}$$

In fact, this allows us to consider the functions u_+, u_- as stricly decreasing in $\pm\infty$ respectively; for instance, thanks to the properties in (3.6) (substituting with $-\omega x, x < 0$ the expression (3.6.2), or in (3.6.7)), a straightforward computation shows that, for $x \to +\infty$, $u_+(x,\lambda)$ behaves like

$$\frac{e^{i\pi/6}}{2\sqrt{\pi}}|x|^{-1/4}e^{i\frac{2}{3}|x|^{3/2}}. \tag{3.2.6}$$

At this point we can extend a solution like u_- on the whole real axis, as solution of the differential equation (3.1.1).

Definition 8.

$$\begin{aligned} v_+ :=& Ai\left(-\frac{\omega^{-1}}{h^{\frac{2}{3}}}(x+\lambda)\right) \text{ for } x > 0 \\ v_- :=& Ai\left(\frac{\omega^{-1}}{h^{\frac{2}{3}}}(x-\lambda)\right) \text{ for } x < 0. \end{aligned} \tag{3.2.7}$$

By the same computation as in (3.2.3), and referring to similar considerations as in (3.2.3) for the function u_+, one can then see that:

Proposition 3.2.4. *The functions $v_\pm$ solve the Schrödinger equation (3.1.1) respectively for $x \gtrless 0$ and they are not vanishing solutions for $x \to \pm\infty$.*

With the previous assumptions, the pair (u_+, v_+) forms, for $\operatorname{Im}\lambda > 0$, a fundamental system for (3.1.1) in $(0, +\infty)$.

Definition 9. Extension of u_- toward $x \geq 0$, as solution of (3.1.1)

$$\widetilde{u}_-(x,\lambda) := \begin{cases} a(\lambda)u_+(x,\lambda) + b(\lambda)v_+(x,\lambda) & x \geq 0 \\ u_-(x,\lambda) & x < 0. \end{cases} \tag{3.2.8}$$

Analogously we define $\widetilde{u}_+(x,\lambda)$:

Definition 10. Extension of u_+ toward $x < 0$, as solution of (3.1.1):

$$\widetilde{u}_+(x,\lambda) := \begin{cases} u_+(x,\lambda) \\ a'(\lambda)u_-(x,\lambda) + b'(\lambda)v_-(x,\lambda) & x < 0. \end{cases} \tag{3.2.9}$$

The previous constructions are defined through analytic continuation and, by applying Airy equation (3.6.1), it is easy to prove as in proposition (3.2.2) that

Proposition 3.2.5. $\widetilde{u}_-(x,\lambda)$ *solves (3.1.1) for* $x \in (-\infty, 0) \cup (0, +\infty)$.

It is well known from the theory of the second order differential equations that the solutions of (3.1.1) should be continuously differentiable on the whole real axis, thus we obtain the following:

Proposition 3.2.6. *Connection formulas:*

1. $u_-(0,\lambda) = \widetilde{u}_-(0,\lambda)$
2. $\partial_x u_-(0,\lambda) = \partial_x \widetilde{u}_-(0,\lambda)$.

The previous condition lead by computation to a linear 2×2 system in two unknowns, $a(\lambda), b(\lambda)$, involving the Wronskian $W(u_+, v_+)$.

Lemma 3.2.7. *Computation of* $b(\lambda)$

$$\begin{aligned}\widetilde{u}_-(0,\lambda) =& a(\lambda)u_+(0,\lambda) + b(\lambda)v_+(0,\lambda) = a(\lambda)Ai\left(-\frac{\omega}{h^{2/3}}\lambda\right) + b(\lambda)Ai\left(-\frac{\omega^{-1}}{h^{2/3}}\lambda\right)\\ \widetilde{u}'_-(0,\lambda) =& a(\lambda)\left(-\frac{\omega}{h^{2/3}}\right)Ai'\left(-\frac{\omega}{h^{2/3}}\lambda\right) + b(\lambda)\left(-\frac{\omega^{-1}}{h^{2/3}}\lambda\right)Ai'\left(-\frac{\omega^{-1}}{h^{2/3}}\lambda\right).\end{aligned} \tag{3.2.10}$$

Thus the connection formulas become:

1. $$\underbrace{Ai\left(-\frac{\omega}{h^{2/3}}\lambda\right)}_{=:A_{11}} = a(\lambda)\underbrace{Ai\left(-\frac{\omega}{h^{2/3}}\lambda\right)}_{=:A_{11}} + b(\lambda)\underbrace{Ai\left(-\frac{\omega^{-1}}{h^{2/3}}\lambda\right)}_{A_{12}}$$
2. $$\underbrace{\frac{\omega}{h^{2/3}}Ai'\left(-\frac{\omega}{h^{2/3}}\lambda\right)}_{=:-A_{21}} = a(\lambda)\underbrace{\left(-\frac{\omega}{h^{2/3}}\right)Ai'\left(-\frac{\omega}{h^{2/3}}\lambda\right)}_{=:A_{21}} + b(\lambda)\underbrace{\left(-\frac{\omega^{-1}}{h^{2/3}}\right)Ai'\left(-\frac{\omega^{-1}}{h^{2/3}}\right)}_{=:A_{22}}.$$

This gives a 2×2 linear system in two unknowns, the coefficients $a(\lambda)$ and $b(\lambda)$, where $A := \left(\begin{smallmatrix} A_{11} & A_{12} \\ A_{21} & A_{22}\end{smallmatrix}\right)$ is the associated matrix. The computation of $det(A) = A_{11}A_{22} - A_{12}A_{21}$, thanks to the properties of the Airy functions, brings to an expression for the Wronskian of v_+ and u_+:

$$W\left(u_+(\cdot,\lambda), v_+(\cdot,\lambda)\right) = -W(v_+, u_+) = -\frac{1}{2\pi i}. \tag{3.2.11}$$

Finally, applying the Cramer rule in order to solve the linear system, we find an expression for the transmission coefficient $b(\lambda)$:

$$b(\lambda) = -2Ai\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)\frac{\omega}{h^{\frac{2}{3}}}Ai'\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right) \cdot 2\pi i. \tag{3.2.12}$$

Remark 3.2.8. Since the definition of $\widetilde{u}_+(0,\lambda)$ is analogously given, it can be shown, that there exist coefficients a' and b' such that $\widetilde{u}_+(x,\lambda)$ solves (3.1.1) on the whole real axis.

Remark 3.2.9. $\widetilde{u}_+, \widetilde{u}_-$ are linearly independent. In fact, let us suppose, that there exists λ, $\operatorname{Im}\lambda > 0$, such that $\widetilde{u}_+, \widetilde{u}_-$ are linearly dependent. For instance, $\widetilde{u}_+ = c\widetilde{u}_-$, where c is some constant. Therefore, we can solve (3.1.1) simultaneously at $\pm\infty$ with a solution u, which actually decays exponentially, in view of the asymptotic behaviour of u_+, u_- (since $\operatorname{Im}\lambda > 0$). It follows that $u \in \mathbf{L}^2(\mathbb{R})$. This is a contradiction: due to the self-adjointness the operator P should only have real eigenvalues, but $\operatorname{Im}\lambda > 0$.

3.2.1 The resolvent kernel

The resolvent kernel is given by:

$$R(x,y,\lambda) = \left(W\left(\widetilde{u}_-, \widetilde{u}_+\right)\right)^{-1} \tilde{u}_-(r_{min},\lambda)\tilde{u}_+(r_{max},\lambda), \tag{3.2.13}$$

where $r_{min} = min\{x,y\}$; $r_{max} = max\{x,y\}$.
In fact, a straightforward computation shows that the integral operator R induced from the kernel maps L^2 into L^2 (for $\operatorname{Im}\lambda > 0$) and satisfies

$$\left(-h^2\partial_x^2 + V - \lambda\right) Ru = u. \tag{3.2.14}$$

Proposition 3.2.10.

$$R(x,y,\lambda) = \left(2Ai\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)\frac{\omega}{h^{\frac{2}{3}}}Ai'\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)\right)^{-1} \widetilde{u}_-(r_{min},\lambda)\widetilde{u}_+(r_{max},\lambda), \tag{3.2.15}$$

and the resonances of P come from zeros of Ai, Ai'.

Proof. By inspection, for fixed x, y, the resolvent kernel has a meromorphic continuation to the complex lower half-plane, thus the resolvent $(P-\lambda)^{-1}$ is an integral operator with kernel R, and has a meromorphic extension too.
Since $W(\widetilde{u}_-, \widetilde{u}_+) = W(au_+ + bv_+, u_+) = b(\lambda)W(v_+, u_+)$, the zeros of $Ai\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)$, $Ai'\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)$ lead to singularities of $R(x,y,\lambda)$, i.e. to resonances of P. □

3.2.2 Expression for the singularities of the resolvent

The zeros of Ai and Ai' are all real and negative, and we can find an expression for the singularities of the resolvent, by computing them from the values of these zeros. The following table contains a list of the first ten zeros of Ai and A':

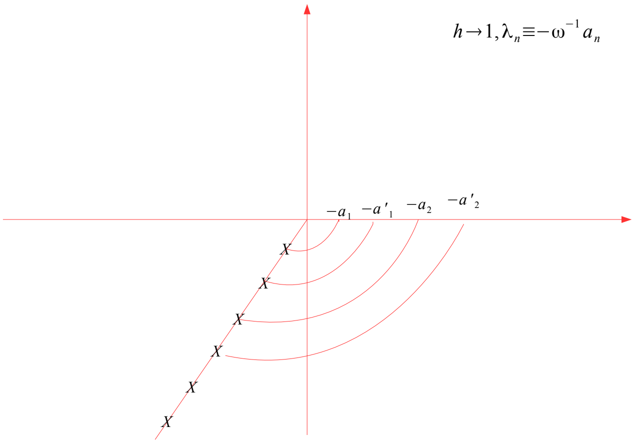


Figure 3.2: Correspondence between resonances and zeros of Airy Function

k	a_k	a'_k
1	-2.33810 74105	-1.01879 29716
2	-4.08794 94441	-3.24819 75822
3	-5.52055 98281	-4.82009 92112
4	-6.78670 80901	-6.16330 73556
5	-7.94413 35871	-7.37217 72550
6	-9.02265 08533	-8.48848 67340
7	-10.04017 43416	-9.53544 90524
8	-11.00852 43037	-10.52766 03970
9	-11.93601 55632	-11.47505 66335
10	-12.82877 67529	-12.38478 83718

By setting

$$-\frac{\omega}{h^{\frac{2}{3}}}\lambda_{2k} = a_k; \ -\frac{\omega}{h^{\frac{2}{3}}}\lambda'_{2k+1} = a'_k \tag{3.2.16}$$

we obtain a simple formula for the resonances:

3.2.3 Resonances

Theorem 3.2.11. *Let a_k, a'_k be the zeros of Ai, Ai' respectively. Then the resonances of the operator P are*

$$Res(P) = \left\{\lambda_k \in \mathbb{C}\ ;\ \lambda_{2k} = -\omega^{-1}h^{\frac{2}{3}}a_k, \quad \lambda_{2k+1} = -\omega^{-1}h^{\frac{2}{3}}a'_k,\ k \in \mathbb{N}\right\}, \tag{3.2.17}$$

and they are localized on a line which is rotated by an angle of $-\frac{2}{3}\pi$ from the real axis.

3.2.4 Analogy with $|x|$

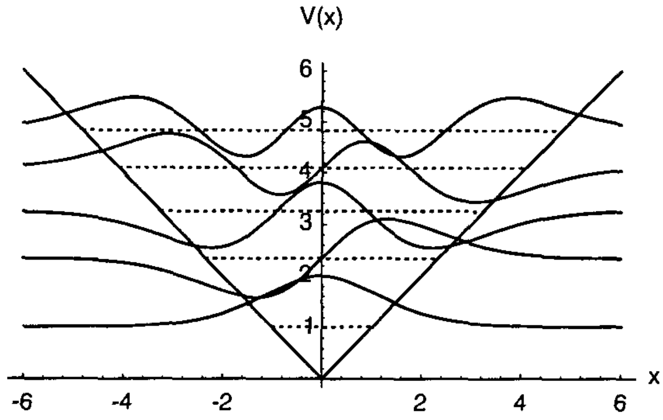


Figure 3.3: First energy levels and corresponding wave functions of $|x|$

The previous resonances are related with the eigenvalues of the Schrödinger operator in the case of a linear potential well $V = |x|$. In that case (see, for instance [VS]), the bound states are determined by solving (3.1.1) for the wave function

$$\psi_n = NAi\left[\left(\frac{2m}{h^2}\right)^{\frac{1}{3}}(|x| - \Lambda_n)\right], \tag{3.2.18}$$

where N is a normalisation constant and Λ_n the energy levels, that are defined by the matching conditions at $x = 0$. According to the parity of the quantum numbers n we obtain two cases.

For example if n is even, the connection formulas enable us to obtain $Ai'[-\Lambda_n] = 0$ (setting $2m = \hbar = 1$ in order to simplify); thus, if a'_n indicates the n^{th} zero of the Ai' function, we will have $\Lambda_n = -a'_{n+1}$ (in a similar way we obtain, for n odd, the value $\Lambda_n = -a_{n+1}$ for the n^{th} zero of the Ai function).

By restoring the constants and computing the normalisation coefficient N, we find an expression for the wave function

$$\psi_n = \left(\frac{2m}{h^2}\right)^{1/6}\frac{1}{\sqrt{-a'_n Ai(a'_n)}}Ai\left[\left(\frac{2m}{h^2}\right)^{1/3}(|x| - \Lambda_n)\right], \tag{3.2.19}$$

i.e. $\Lambda_n = -a'_{n+1}\left(\frac{h^2}{2m}\right)^{1/3}$, which is very similar to that of the resonances of the previous section.

3.3 Linear wedge without symmetry

We want to slightly generalize the form of the potential, assuming for instance,

$$V(x,\alpha) := \begin{cases} -\alpha x & x \geq 0, \alpha > 0, \\ x & x < 0. \end{cases} \tag{3.3.1}$$

As in the section (3.2) we can construct a function

$$u_+ := Ai\left(-\frac{\omega}{(\alpha h)^{\frac{2}{3}}}(\alpha x + \lambda)\right), \tag{3.3.2}$$

that solves the Schrödinger equation (3.1.1). The behavior of other solution as in definition (8) and (9) can be analogously determined, and all the computations (Wronskian, connection formulas, etc.) are very similar to the ones of section (3.2), although the lack of symmetry gives rise to a different expression for the transmission coefficient, more complicated. In fact, the resonances turn out to be zeros of this expression:

$$\left[Ai\left(-\frac{\omega}{(\alpha h)^{\frac{2}{3}}}\lambda\right)Ai'\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right) + \alpha^{\frac{1}{3}}Ai'\left(-\frac{\omega}{(\alpha h)^{\frac{2}{3}}}\lambda\right)Ai\left(-\frac{\omega}{h^{\frac{2}{3}}}\lambda\right)\right]. \tag{3.3.3}$$

To analyze these zeros one could consider the self-adjoint operator $P = -h^2\partial_x^2 - V(x)$; similarly to the symmetric case of section (3.2), there is an increasing sequence of real numbers $c_k, k \in \mathbb{N}$, such that

$$\sigma(P) = \{h^{\frac{2}{3}}c_k; k \in \mathbb{N}\}. \tag{3.3.4}$$

The numbers c_k are the zeros of

$$\left[Ai\left(-\frac{\lambda}{(\alpha h)^{\frac{2}{3}}}\right)Ai'\left(-\frac{\lambda}{h^{\frac{2}{3}}}\right) + \alpha^{\frac{1}{3}}Ai'\left(-\frac{\lambda}{(\alpha h)^{\frac{2}{3}}}\right)Ai\left(-\frac{\lambda}{h^{\frac{2}{3}}}\right)\right]. \tag{3.3.5}$$

In particular (since the zeros correspond to eigenvalues of the self-adjoin operator, which spectrum consists of real and positive numbers), this proves that all zeros of this combination of Airy functions are real and positive.
It follows that all the resonances of $P = -h^2\partial_x^2 + V(x)$ are of the form

$$\omega^{-1}h^{\frac{2}{3}}c_k(\alpha). \tag{3.3.6}$$

3.3.1 Tunneling without any symmetry

We consider now a linear potential whit a different slope for $x > 0$ and $x < 0$.

Definition 11.

$$V_0(x) = V(x; \alpha_1, \alpha_2) := \begin{cases} -\alpha_2 x & x \geq 0, \\ \alpha_1 x & x < 0 \quad (\alpha_1, \alpha_2) > 0. \end{cases} \tag{3.3.7}$$

Proposition 3.3.1.

$$u_+(x, \lambda) := Ai(-\frac{\omega}{(\alpha_2 h)^{2/3}}(\alpha_2 x + \lambda)) \tag{3.3.8}$$

$$\textit{solves } (-h^2\partial_x^2 - \alpha_2 x - \lambda)u_+(x, \lambda) = 0 \quad \textit{for } x \geq 0. \tag{3.3.9}$$

As in the previous section, all the definition and the conditions that lead to an expression for the resonances, are in fact directly related with the computations in (3.2).

They bring us to the following form for the transmission coefficient:

$$\begin{aligned} b(\lambda) = \alpha_b \left(\frac{\alpha_1}{\alpha_2}\right)^{1/3} Ai'\left(-\frac{\omega}{(\alpha_1 h)^{2/3}}\lambda\right) Ai\left(-\frac{\omega}{(\alpha_2 h)^{2/3}}\lambda\right) \\ +\alpha_b Ai'\left(-\frac{\omega}{(\alpha_2 h)^{2/3}}\lambda\right) Ai\left(-\frac{\omega}{(\alpha_1 h)^{2/3}}\lambda\right), \end{aligned} \tag{3.3.10}$$

where $\alpha_b = \dfrac{\omega}{h^{2/3}\alpha_2^{1/3}}$.
Alternatively the computation of the resonances can be reduced to the case $\alpha_1 = 1$ considered above. There is an increasing sequence of positive real numbers $\widetilde{c}_k$ such that the resonances are of the form $\omega^{-1}h^{\frac{2}{3}}\widetilde{c}_k,\ k \in \mathbb{N}$. Here the values $\widetilde{c}_k(\alpha_1, \alpha_2)$ are given by

$$\widetilde{c}_k(\alpha_1, \alpha_2) = \alpha_1^{\frac{2}{3}} c_k(\frac{\alpha_1}{\alpha_2}), \tag{3.3.11}$$

where the $c_k(\alpha)$'s are the numbers mentioned in the section (3.3), setting $\alpha = \frac{\alpha_2}{\alpha_1}$;

In fact, writing $\widetilde{P} = -h^2\partial_x^2 - V(x; \alpha)$, it follows

$$\begin{aligned} \widetilde{P} = \alpha_1 \left[-\left(\frac{h}{\sqrt{\alpha_1}}\right)^2 \partial_x^2 - V(x, \alpha)\right]; \\ \sigma(\widetilde{P}) = \alpha_1 \sigma \left[\left(\frac{h}{\sqrt{\alpha_1}}\right)^2 \partial_x^2 - V(x, \alpha)\right]. \end{aligned} \tag{3.3.12}$$

Thus, by shifting the factor which contains h, α_1, it comes out formula (3.3.11). Analogously, analysing the operator $\widetilde{P}$ with a plus sign of the potential as in (3.3), the resonances will be of the form

$$\omega^{-1}h^{\frac{2}{3}}\widetilde{c}_k(\alpha_1, \alpha_2). \tag{3.3.13}$$

3.4 Main result

Consider the potential $V = V_1$ in $x < 0, V = V_2$ in $x \geq 0$, where

- V_j are analytic in regions Γ_j,

$$\Gamma_{1,2} := \{x \in \mathbb{C}; |\text{Im}\, x| < \delta_0 \langle \text{Re}\, x \rangle\} \cap [\mp \text{Re}\, x > -\delta_1], \tag{3.4.1}$$

  for some $\delta_j > 0$;

- there are constants $V_1^-, V_2^+ < 0$:

$$V_1(x) \to V_1^- \qquad (\text{Re}\, x \to -\infty \quad \text{in} \quad \Gamma_1); \tag{3.4.2}$$

$$V_2(x) \to V_2^+ \qquad (\text{Re}\, x \to \infty \quad \text{in} \quad \Gamma_2), \tag{3.4.3}$$

and V is a real valued continuous function on the real line satisfying

$$V(x) < 0 \quad (x \in \mathbb{R} \setminus 0), \qquad V(0) = 0, \tag{3.4.4}$$

with linearization $V_0(x) = V(x; \alpha_1, \alpha_2)$ at $x = 0$, i.e.:

$$V_0(x) = \alpha_1 x \quad (x < 0), V_0(x) = -\alpha_2 x \quad (x > 0), \tag{3.4.5}$$

for some $\alpha_j > 0$, $(j = 1, 2)$.

3.4.1 Set of resonances

Theorem 3.4.1.

$$\textit{Set} \quad D_h(C_0) = \left[-C_0 h^{2/3}, C_0 h^{2/3}\right] - i \left[0, C_0 h^{\frac{2}{3}}\right]. \tag{3.4.6}$$

Then for any $C_0 > 0$, h sufficiently small, the operator $P = -h^2 \partial_x^2 + V(x)$ has resonances

$$\textit{Res}(P) \cap D_h(C_0) = \{\lambda_k(h); k \in \mathbb{N}\} \cap D_h(C_0), \tag{3.4.7}$$

$$\textit{where} \quad \lambda_k(h) \sim h^{\frac{2}{3}} \sum_n c_{k,n} h^{\frac{n}{3}}. \tag{3.4.8}$$

The leading term $\lambda_{k,0}(h) = h^{2/3} c_{k,0}$ coincides with the resonances for the linearized operator $P_0 = -h^2 \partial_x^2 + V_o$.

Proof. We write the proof for $\alpha_1 = \alpha_2 = 1$ only, since the general case can be deduced in a straightforward way.

We proceed in a way very similar to that of [FMW]. First of all, following the constructions of [FMW], Appendix, for $E \in D_h(C_0)$, we can construct two functions

u_1 and u_2, defined on $I_1 := (-\infty, \delta_1]$ and $I_2 := [-\delta_1, +\infty)$ respectively, that are solutions to,

$$-h^2 u_j'' + V_j u_j = E u_j \quad \text{on } I_j \quad (j = 1, 2),$$

and such that,

$$u_1 = \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (E - V_1(x))^{-1/4} e^{-i \int_{x_1(E)}^{x} \sqrt{E - V_1(t)}\, dt/h} (1 + o(1)) \quad (x \to -\infty);$$
$$u_2 = \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (E - V_2(x))^{-1/4} e^{i \int_{x_2(E)}^{x} \sqrt{E - V_2(t)}\, dt/h} (1 + o(1)) \quad (x \to +\infty),$$

where $x_j(E)$ stands for the unique complex point near 0 where $V_j - E$ vanishes.

In particular, u_1 (resp. u_2) is out-going at $-\infty$ (resp. $+\infty$), and $E \in D_h(C_0)$ will be a resonance of P iff there exists a (continuously differentiable) solution $u \neq 0$ to $Pu = Eu$, such that u is both proportional to u_1 on $(-\infty, 0]$ and to u_2 on $[0, +\infty)$. But this is equivalent to the fact that the Wronskian of u_1 and u_2 vanishes at 0. Therefore, the quantization condition simply reads,

$$u_1(0) u_2'(0) - u_1'(0) u_2(0) = 0. \tag{3.4.9}$$

(In this case, setting $\beta := u_1(0)/u_2(0) = u_1'(0)/u_2'(0)$, the resonant state u will be given by $u = u_1$ on $(-\infty, 0]$, and $u = \beta u_2$ on $[0, +\infty)$.)

In order to solve (3.4.9), we use a semiclassical asymptotic expansions of u_1 and u_2 near 0. We set,

$$f_j(h^{-\frac{2}{3}} \xi_j(x)) := \xi_j'(x)^{\frac{1}{2}} u_j(x),$$

where $\xi_j(x)$ is the analytic continuation to complex values of E of the function, originally defined for real values of E,

$$\xi_j(x; E) = -\left(\frac{3}{2} \int_x^{x_j(E)} \sqrt{V_j(t) - E\, dt} \right)^{\frac{2}{3}} \quad \text{when } x \in \Gamma_j.$$

Then, by [FMW], Section 8 and [Y], we have,

$$f_1 = (\mathrm{Ai} - i\mathrm{Bi}) \sum_{k=0}^{\infty} L_1^k(\mathbf{1});$$
$$f_2 = (\check{\mathrm{A}}\mathrm{i} - i\check{\mathrm{B}}\mathrm{i}) \sum_{k=0}^{\infty} L_2^k(\mathbf{1}),$$

where $\mathbf{1}$ stands for the constant function of value 1, and the operators L_1 and L_2 are defined on the set $C_b(\mathbb{R}_\pm)$ of bounded continuous functions on $\mathbb{R}_\pm$ respectively, by the formulas,

$$L_1 g(t) := \int_0^t \frac{A_{out}^-(s)}{A_{out}^-(t)} \left(\mathrm{Ai}(t)\mathrm{Bi}(s) - \mathrm{Bi}(t)\mathrm{Ai}(t)(s)\right) R_1(s) g(s) ds \quad (t \leq 0);$$
$$L_2 g(t) := \int_0^t \frac{A_{out}^+(s)}{A_{out}^+(t)} \left(\check{\mathrm{Ai}}(t)\check{\mathrm{Bi}}(s) - \check{\mathrm{Bi}}(t)\check{\mathrm{Ai}}(t)(s)\right) R_2(s) g(s) ds \quad (t \geq 0),$$

where $A_{out}^- := \mathrm{Ai} - i\mathrm{Bi}$, $\check{\mathrm{Ai}}(\mathrm{t}) = \mathrm{Ai}(-\mathrm{t}), \check{\mathrm{Bi}}(\mathrm{t}) = \mathrm{Bi}(-\mathrm{t})$, $A_{out}^+ := \check{\mathrm{Ai}} - i\check{\mathrm{Bi}}$, $R_j(s) := h^{4/3}\sigma_j(h^{2/3}s)$, $\sigma_j(x) := \left[(\xi_j'(x))^{-1/2}\right]''(\xi_j'(x))^{-3/2}$.

In particular, on can show that the norms of L_j are $\mathcal{O}(h)$, and since ξ_j is analytic at 0, we see that, actually, $u_j(0)$ and $h^{2/3}u_j'(0)$ admit complete asymptotic expansions in powers of $h^{\frac{1}{3}}$, with coefficients depending analytically on $\rho := Eh^{-2/3}$. Their leading terms are given by,

$$u_1(0) = A_{out}^-(-\rho) + \mathcal{O}(h^{\frac{1}{3}});$$
$$h^{2/3}u_1'(0) = (A_{out}^-)'(-\rho) + \mathcal{O}(h^{\frac{1}{3}});$$
$$u_2(0) = A_{out}^+(\rho) + \mathcal{O}(h^{\frac{1}{3}}) = A_{out}^-(-\rho) + \mathcal{O}(h^{\frac{1}{3}});$$
$$h^{2/3}u_2'(0) = (A_{out}^+)'(\rho) + \mathcal{O}(h^{\frac{1}{3}}) = -(A_{out}^-)'(-\rho) + \mathcal{O}(h^{\frac{1}{3}}).$$

Therefore, at the first order in $h^{\frac{1}{3}}$, the quantization condition becomes,

$$A_{out}^-(-\rho)(A_{out}^-)'(-\rho) = \mathcal{O}(h^{\frac{1}{3}}).$$

In fact, observing the behaviour of the Airy functions Ai, Bi at infinity, it turns out that $A_{out}^- = \frac{e^{-i\pi/3}}{2} Ai(\omega x)$ as stated in (3.6.6; this means that also their zeros correspond, and the quantization condition leads to computations that are related to the ones in the previous sections.

We deduce that $\rho = \rho_0 + \mathcal{O}(h^{\frac{1}{3}})$ with $\rho_0 \in \{z \in \mathbb{C}\,;\, A_{out}^-(-z)(A_{out}^-)'(-z) = 0\} = \{-\omega^{-1}a_k\,;\, k \geq 1\} \cup \{-\omega^{-1}a_k'\,;\, k \geq 1\}$. Then, using the analyticity of all the coefficients with respect to ρ, we conclude in a standard way the existence of complete asymptotic expansions of ρ in powers of $h^{\frac{1}{3}}$. In fact, all this can be made explicit by use of Lagrange's inversion formula (in a version for formal power series). For a proof see e.g. [WW].

Writing $F(\rho, h) = u_1(0)u_2'(0) - u_1'(0)u_2(0)$, we have, by the WKB expansion constructed above,

$$F(\rho, h) = \sum_{k=0}^{\infty} c_k(\rho) h^{k/3}, \tag{3.4.10}$$

with coefficients c_k analytic in ρ. If $c_0(\rho_0) = 0$, i.e. ρ_0 corresponds to one of the resonances of the linear wedge problem as described above, we know from the properties of the Airy function (or, in the case of a non-symmetric linear wedge, from properties of the solutions of a Sturm Liouville problem) that it is a simple zero, leading to $F'(\rho_0, h) \neq 0$. Furthermore $F(\rho_0, h) = O(h^{1/3})$ is a formal power series in $h^{1/3}$.

Then the Lagrange inversion formula represents the unique zero ρ of $F(\cdot, h)$ close to ρ_0 by the explicit formula

$$\rho = \rho_0 + \sum_{n=1}^{\infty} \frac{(-1)^n F(\rho_0, h)^n}{n!} \lim_{w \to \rho_0} \partial_w^{n-1} \left(\frac{w - \rho_0}{F(w,h) - F(\rho_0, h)} \right)^n . \qquad (3.4.11)$$

Clearly, this formal sum of formal power series defines by ordering according to powers of $h^{1/3}$ a complete asymptotic expansion, as claimed above. While the classical form of the Lagrange inversion formula refers to analytic functions $F(\rho)$, our version of the formula for formal power series in $h^{1/3}$ follows immediately from the classical result replacing $F(\rho, h)$ by finite partial sums. This proves our theorem.

□

Remark: This result probably extends to potentials $V(x) \sim \alpha_{\pm} x$ at $x \to \pm\infty$. But this needs a different WKB construction. We expect that this type of result appears in the Born-Oppenheimer approximation. The purpose is to extend the previous constructions for the two-level problem with a crossing as in [FMW],

$$H(x) := \begin{pmatrix} -h^2\Delta + V_1 & hR \\ h\overline{R} & -h^2\Delta + V_2 \end{pmatrix} \qquad (3.4.12)$$

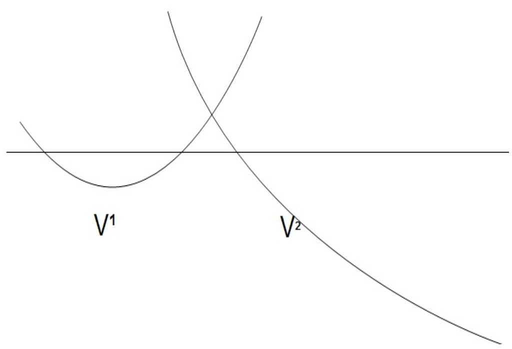


Figure 3.4: 2-level Potential with crossing

This could be done thanks to the analogy between the linear wedge barrier and the crossing between the two potential , V_1, V_2; As in Theorem 2.1 of [FMW] the resonances E_k for $h > 0$ small enough has Im $E_k \sim h^{\frac{5}{3}}$ in first approximation, and the previous resonances are connected with the bound trajectory of a particle in the potential V_1. They are longer lived than resonances due to the linear wedge alone. (Who would be sitting on a wedge?) In the B-O approximation, in a window Im $\lambda \in [-ch^{\frac{2}{3}}, 0]$, we expect to find resonances with a similar construction of the scalar case in the matrix case. But the full construction needs a new idea compared with the work of A.Martinez et al.([FMW]).

Appendix

3.5 Semiclassical Pseudodifferential Calculus

3.5.1 Spaces of Symbols

Definition 12. An order function is a function $g \in C^{\infty}(\mathbb{R}^n, \mathbb{R}^+)$ such that $\partial_x^{\alpha} = \mathcal{O}(g)$ for any $\alpha \in \mathbb{N}^n$ uniformly on $\mathbb{R}^n$.

We denote by $\langle \xi \rangle$ the order function $\sqrt{1 + |\xi|^2}$.

Definition 13. Let $a = a(x, \xi) \in \mathbf{C}^{\infty}(\mathbb{R}^{2n})$; a is said to be a symbol of order m ($m \in \mathbb{R}$ fixed), denoted by $a \in \mathbf{S}(\langle \xi \rangle^m)$ if, for any $\alpha \in \mathbb{N}^{2n}$, there exists $C_{\alpha} > 0$ such that

$$|\partial^{\alpha} a(x, \xi)| \leqslant C_{\alpha} \langle \xi \rangle^m \quad \forall\, (x, \xi) \in \mathbb{R}^{2n}$$

.

Example 4. If $\chi \in \mathbf{C}_0^{\infty}(\mathbb{R}^{2n}) \implies \chi \in \mathbf{S}(1) \equiv \mathbf{S}(\langle \xi \rangle^0)$.

Example 5. If $V(x) \in \mathbf{S}(1) \implies \xi^2 + V(x) \in \mathbf{S}(\langle \xi \rangle^2)$.

Example 6. $\forall m \in \mathbb{R}\ \langle \xi \rangle^m \in \mathbf{S}(\langle \xi \rangle^m)$.

Proposition 3.5.1.

$$m, m^1 \in \mathbb{R}\,, a \in \mathbf{S}(\langle \xi \rangle^m), b \in \mathbf{S}(\langle \xi \rangle^{m^1}) \Longrightarrow ab \in \mathbf{S}(\langle \xi \rangle^{m+m^1})$$

Definition 14. A symbol $a \in \mathbf{S}(\langle \xi \rangle^m)$ is said to be elliptic in $\mathbf{S}(\langle \xi \rangle^m)$ if there exists a constant $C > 0$ such that, for any $(x, \xi) \in \mathbb{R}^{2n}$

$$|a(x, \xi)| \geq \frac{1}{C} \langle \xi \rangle^m. \tag{3.5.1}$$

Example 7. $\langle \xi \rangle^m$ is elliptic in $\mathbf{S}(\langle \xi \rangle^m)$.

Example 8. If $V \in \mathbf{S}(1)$ is such that $\inf_{\mathbb{R}^n} V > 0$, then $\xi^2 + V(x)$ is elliptic in $\mathbf{S}(\langle \xi \rangle^2)$.

Proposition 3.5.2. *Let a be elliptic in $\mathbf{S}(\langle\xi\rangle^m)$. Then $\frac{1}{a} \in \mathbf{S}(\langle\xi\rangle^{-m})$*

Definition 15. Let $a(x,\xi;h)$ (semiclassical symbol, depending on h) be $\in \mathbf{S}(\langle\xi\rangle^m)$. Let $a_0, a_1 \ldots$ be a sequence of symbols of $\mathbf{S}(\langle\xi\rangle^m)$. Then we say that a is asymptotically equivalent to the formal sum $\sum_{j\geq 0} h^j a_j$ in $\mathbf{S}(\langle\xi\rangle^m)$ (notation: $a \sim \sum_{j\geq 0} h^j a_j$) if and only if for any $N \geq 1$, $\alpha \in \mathbb{N}^{2n}$, there exists a constant $C(\alpha, N) > 0$, such that

$$|\partial^\alpha\big(a(x,\xi) - \sum_{j=0}^{N} h^j a_j(x,\xi)\big)| \leq Ch^N \langle\xi\rangle^m, \tag{3.5.2}$$

for $h > 0$ small enough.

In the particular case where all the symbols are identically zero, $a_j = 0\,\forall\, j$, we write $a \sim 0$ in $\mathbf{S}(\langle\xi\rangle^m)$, or $a = \mathcal{O}(h^\infty)$ in $\mathbf{S}(\langle\xi\rangle^m)$.

Remark 3.5.3. Let $(a_j)_{j\geq 0}$ be an arbitrary sequence of $\mathbf{S}(\langle\xi\rangle^m)$. Then there exists $a \in \mathbf{S}(\langle\xi\rangle^m)$ such that $a \sim \sum_{j\geq 0} h^j a_j$ in $\mathbf{S}(\langle\xi\rangle^m)$. Moreover a is unique up to $\mathcal{O}(h^\infty)$.
Such a symbol a is called *RESUMMATION* of $\sum_{j\geq 0} h^j a_j$ in $\mathbf{S}(\langle\xi\rangle^m)$.

A useful application is the WKB method (Wentzel, Kramer, Brillouin), used to construct approximate solutions of the one-dimensional Schrödinger equation of the form
$u(x;h) = e^{i\varphi(x)/h} \sum_{j\geq 0} h^j a_j$.

3.5.2 Semiclassical pseudodifferential operators

Proposition 3.5.4. *Let $m \in \mathbb{R}, a \in \mathbf{S}(\langle\xi\rangle^m), a = a(x,y,\xi)$ The semiclassical pseudodifferential operator of symbol a of degree m is an operator that maps $u \in \mathcal{S}(\mathbb{R}^n)$ to the function*

$$Op_h(a)u(x;h) = \frac{1}{(2\pi h)^n} \int\int e^{i(x-y)\xi/h} a(x,y,\xi)u(y)dyd\xi, \tag{3.5.3}$$

in the sense of oscillatory integrals. Therefore, for any $a \in \mathbf{S}(\langle\xi\rangle^m)$, $Op_h(a)$ maps $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}(\mathbb{R}^n)$.

If $a \in \mathbf{S}(\langle\xi\rangle^m), d \in \mathbb{R}$, then we denote by

$$h^{-d} Op_h(a) \tag{3.5.4}$$

the operator of degree m and order d.

Example 9. (Semiclassical differential operators)
In the particular case where a is of the form:

$$a(x,y,\xi) = \sum_{|\alpha|\leq m} b_\alpha(x)\xi^\alpha, \tag{3.5.5}$$

with $b_\alpha \in \mathbf{S}(1)$, we obtain

$$Op_h(\sum_{|\alpha|\leq m} b_\alpha(x)\xi^\alpha) = \sum_{|\alpha|\leq m} b_\alpha(x)(hD_x)^\alpha. \tag{3.5.6}$$

Example 10. (Usual differential operators)
If the symbols $b_\alpha \in \mathbf{S}(1)$, the differential operator

$$P = \sum_{|\alpha|\leq m} b_\alpha(x)D_x^\alpha \tag{3.5.7}$$

can be rewritten as

$$P = h^{-m}\sum_{j=0}^{m} h^j \sum_{|\alpha|=m-j} b_\alpha(hD_x)^\alpha, \tag{3.5.8}$$

Then P becomes a semiclassical pseudodifferential operator of order m. Its corresponding symbol will be

$$p(x,\xi;h) = h^{-m}\sum_{j=0}^{m} h^j p_j(x,\xi), \tag{3.5.9}$$

where $p_j(x,\xi) = \sum_{|\alpha|=m-j} b_\alpha(x)\xi^\alpha$.

Note that the composition of such operators is well defined, although there is not uniqueness of the symbol for a pseudodifferential operator (Composition theorem 2.6.5, [Ma2]). (For instance, if $n=1$ we have $Op_h(x\xi) = Op_h(y\xi + ih)$, or $x \cdot hD_x$ and $hD_x \cdot x - \frac{h}{i}$ correspond).
To overcome this ambiguity we introduce the "Weyl quantization":

$$Op_h^W \equiv Op_h^{1/2}(a) := Op_h(a(\frac{x+y}{2},\xi)), \tag{3.5.10}$$

which is a particular case of the general definition of "t-quantization" of a,

$$Op_h^t := Op_h\big(a((1-t)x + ty,\xi)\big),\ t \in [0,1], \tag{3.5.11}$$

where it can be proved that makes the symbol unique. Namely, in order to simplify the computations it is better to remain in a given quantization (a fixed value of t), and this is possible thanks to the existence of a unique symbol $b_t(x,\xi) \in \mathbf{S}_{2n}(\langle\xi\rangle^m)$ depending on $2n$ variables only, that can be associated to $b(x,y,\xi) \in$

$\mathbf{S}_{3n}(\langle\xi\rangle^m)$ because of theorem 2.7.1 in [Ma2].

Thanks to this powerful tool we can write the Schrödinger operator as a pseudodifferential operator of symbol $\xi^2 + V(x)$. Moreover, if the symbol a is real valued, Op_h^W turns out to be formally sef-adjoint, i.e. symmetric with respect to the scalar product in $\mathbf{L}^2(\mathbb{R}^n)$; this is very useful in quantum mechanics.

3.5.3 Symbolic Calculus: some general results in the case of Weyl quantization

Thanks to the uniqueness of the symbol by the composition of pseudodifferential operators, following theorem 2.7.4 in [Ma2], we introduce the "Moyal product": , $\exists!\, c(x,\xi) \in \mathbf{S}(\langle\xi\rangle^{m+m'})$ such that

$$Op_h^W(a) \circ Op_h^W(b) = Op_h^W(c), \tag{3.5.12}$$

setting

$$c = a\sharp^W b. \tag{3.5.13}$$

Theorem 3.5.5. $\forall a \in \mathbf{S}(\langle\xi\rangle^m), \forall b \in \mathbf{S}(\langle\xi\rangle^{m'})$ *holds:*

$$(a\sharp^W b)(x,\xi) \sim \sum_k \frac{h^k}{i^k k!}\big(\nabla_\eta\nabla_z - \nabla_\xi\nabla_y\big)^k \cdot \big[a\big((1+t)x+ty,\eta\big)\cdot b\big(tx+(1-t)z,\xi\big)\big]|_{\substack{y=z=x\\ \eta=\xi}} \tag{3.5.14}$$

in $\mathbf{S}(\langle\xi\rangle^{m+m'})$.

Remark 3.5.6. In first approximation the previous composition corresponds to the multiplication of the symbols:

$$(a\sharp^W b)(x,\xi) = a(x,\xi)b(x,\xi) + \mathcal{O}(h) \text{ in } \mathbf{S}(\langle\xi\rangle^{m+m'}); \tag{3.5.15}$$

moreover,

$$\begin{aligned} a\sharp^W b &\sim \sum_{\alpha,\beta\in\mathbb{N}^m} \frac{(-1)^{|\alpha|}h^{|\alpha-\beta}}{(2i)^{|\alpha+\beta|}\alpha!\beta!}\big(\partial_x^\alpha\partial_\xi^\beta a\big)\big(\partial_x^\beta\partial_\xi^\alpha b\big) = \\ &= ab + \frac{h}{2i}\big(\nabla_\xi a\nabla_x b - \nabla_x a\nabla_\xi b\big) + \mathcal{O}(h^2) \text{ in } \quad \mathbf{S}(\langle\xi\rangle^{m+m'}) = \\ &= ab + \frac{h}{2i}\{a,b\} + \mathcal{O}(h^2). \end{aligned} \tag{3.5.16}$$

where $\{a,b\}$ represents the Poisson brackets of a, b.

Theorem 3.5.7. *(Calderón-Vaillancourt)*
Let $a \in \mathcal{S}(1)$. Then the operator $Op_h(a)$ is continuous on $\mathbf{L}^2(\mathbb{R}^n)$ and

$$\|Op_h(a)\|_{\mathcal{L}(L^2)} \le C_n\Big(\sum_{|\alpha|\le M_n}\|\partial^\alpha a\|_{L^\infty(\mathbb{R}^{3n})}\Big), \tag{3.5.17}$$

where the positive constants M_n, C_n depend only on n.

Furthermore:

Theorem 3.5.8. *Let a be in $\mathcal{S}_{2n}(1)$ such that, for any $\alpha \in \mathbb{N}^{2n}$*

$$\partial^\alpha a(x,\xi) \to 0 \text{ for } |(x,\xi)| \to +\infty. \tag{3.5.18}$$

Then the operator $A := Op_h^W(a)$ is compact on $\mathbf{L}^2(\mathbb{R}^n)$.

In the case $a \in \mathcal{S}_{3n}(1)$, considering the operator $Op_h(a)$, by integration by part in the area $|x-y| \geq \delta|x|$ (for some $\delta > 0$), a sufficient assumption for the compactness of $Op_h(a)$ is the existence of $\delta_1 > 0$ such that, for any $\alpha \in \mathbb{N}^{3n}$,

$$\partial^\alpha a(x,y,\xi) \longrightarrow 0 \quad \text{for} \quad \begin{cases} |(x,y,\xi)| \to \infty \\ |x-y| \leq \delta_1|x| \end{cases}. \tag{3.5.19}$$

Definition 16. For $u(x,h) \in S'(\mathbb{R}^n)$, we define the so-called *FBI-Bargmann transform T* by the formula,

$$Tu(x,\xi;h) = 2^{-\frac{n}{2}}(\pi h)^{-\frac{3n}{4}} \int_{\mathbb{R}^n} e^{i(x-y)\xi/h-(x-y)^2/2h}u(y,h)dy, \tag{3.5.20}$$

used by many authors ([Ma2], [Sj]) to treat simultaneously the local behavior of u and that of its h-Fourier transform $\mathcal{F}_h u$.

From the theory of such operators we can derive characteristics of u just by knowing the behavior of Tu; its local properties are called *microlocal* properties of u, and the fact that $Tu = \mathcal{O}(h^\infty)$ near some point (x_0,ξ_0) will be expressed by saying that u is *microlocally* $\mathcal{O}(h^\infty)$ near that point.

Definition 17. For $u(x,h) \in S'(\mathbb{R}^n)$, $(x_0,\xi_0) \in \mathbb{R}^{2n}$, we say that u is microlocally exponentially small near (x_0,ξ_0) if there exists some $\delta > 0$ such that

$$Tu(x,\xi;h) = \mathcal{O}(e^{-\delta/h}),$$

uniformly for (x,ξ) in a neighborhood of (x_0,ξ_0). The complementary set of such points (x_0,ξ_0) is called the "microsupport" of u, and is denoted $MS(u) \subset \mathbb{R}^{2n}$. In other words, it is the subset of $\mathbb{R}^{2n}$ consisting of the points near which u is not microlocally exponentially small as $h \to 0$.
The properties of invariance for the microsupport are a useful tool to studying solutions of analytic PDEs. They are related to the geometry of the characteristic set of the equation; in fact, the microsupport of a solution of a PDE is invariant by the Hamilton flow associated with the equation, i.e. any point of the microsupport gives rise to a whole curve passing through this point and contained in the microsupport (propagation of the microsupport).

3.6 Airy functions

The behavior of the Airy functions is oscillatory at $x \to -\infty$ and exponential at $x \to \infty$. They are the most basic functions that exhibit a transition from oscillatory to exponential behavior, and because of this they arise in many applications, for instance in describing waves at caustics or turning points (see e.g. [O]). The Airy function $Ai(x), x \in \mathbb{R}$ is characterised as the solution to the homogeneus second order differential equation (called the Airy equation)

$$u''(x) = xu(x). \tag{3.6.1}$$

It decays exponentially as $x \to +\infty$:

$$Ai(x) \sim \frac{1}{2\sqrt{\pi}} x^{-\frac{1}{4}} e^{-\frac{2}{3}x^{3/2}}; \tag{3.6.2}$$

When $x < 0$ it is oscillating and at $x \to -\infty$ it behaves as:

$$Ai(x) \sim \frac{1}{\sqrt{\pi}} (-x)^{-\frac{1}{4}} \sin\left(\frac{2}{3}(-x)^{3/2} + \frac{\pi}{4}\right). \tag{3.6.3}$$

Moreover, the asymptotic behaviour of its derivative Ai' is obtained by formally differentiating the previous one, and these asymptotic behaviors remain valid in sufficiently small complex sectors around the real line.
We define as further solution of the equation (3.6.1) the function $Bi(x)$, (which has the interesting property to be real when x is real), linearly independent of $Ai(x)$, by the asymptotic behavior as $x \to -\infty$:

$$Bi(x) \sim \frac{-1}{\sqrt{\pi}} (-x)^{-\frac{1}{4}} \sin\left(\frac{2}{3}(-x)^{3/2} - \frac{\pi}{4}\right). \tag{3.6.4}$$

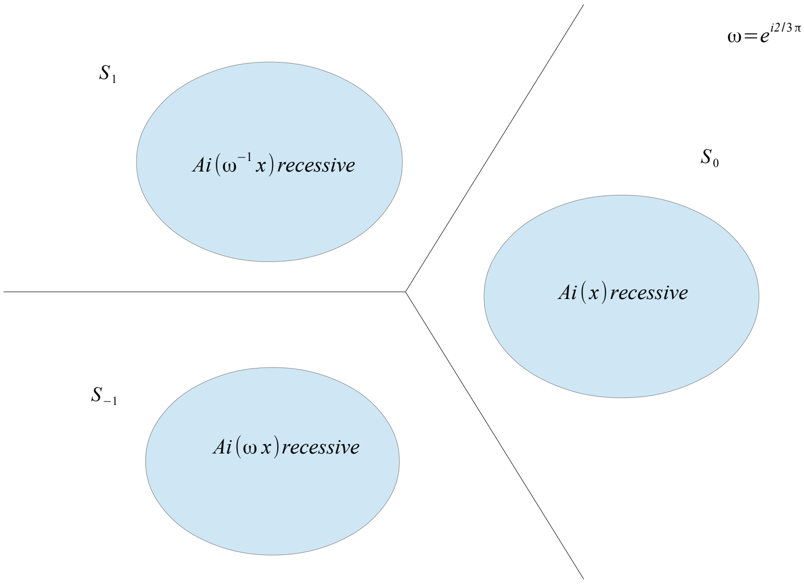
$Bi(x)$ is positive and grows exponentially for $x > 0$, and satisfies for $x \to +\infty$:

$$Bi(x) \sim \frac{1}{\sqrt{\pi}} x^{-\frac{1}{4}} e^{\frac{2}{3}x^{3/2}}. \tag{3.6.5}$$

Other solutions of the Airy equation are $Ai(x\omega^{\pm 1})$, where $\omega := e^{i\frac{2}{3}\pi}$ $(1, \omega, \omega^2$ are the cubic roots of the unity);

From standard properties we deduce the following relations between Airy functions:

$$\begin{aligned} Ai(\omega^{\pm 1}x) &= \frac{e^{\pm i\frac{\pi}{3}}}{2}[Ai(x) \mp iBi(x)]; \\ Ai'(\omega^{\pm 1}x) &= \frac{e^{\mp i\frac{\pi}{3}}}{2}[Ai'(x) \mp iBi'(x)]; \\ Bi(x) &= e^{i\frac{\pi}{6}} Ai(\omega x) + e^{-i\frac{\pi}{6}} Ai(\omega^{-1}x); \\ Bi'(x) &= e^{i\frac{5\pi}{6}} Ai'(\omega x) + e^{-i\frac{5\pi}{6}} Ai'(\omega^{-1}x). \end{aligned} \tag{3.6.6}$$



Moreover, from the asymptotic behaviors of $Ai(x)$ and $Bi(x)$ as $x \to -\infty$, one can easily see the following properties:

$$\begin{aligned} Ai(x) - iBi(x) &\sim \frac{e^{-i\frac{\pi}{4}}}{\sqrt{\pi}}(-x)^{-\frac{1}{4}} exp\left(\frac{2i}{3}(-x)^{\frac{3}{2}}\right); \\ Ai(\omega x) = o(1) \quad in \quad & S_{-1} := \{z \in \mathbb{C} / -\pi \leq |\arg(z)| \leq -\frac{\pi}{3}\}; \\ Ai(\omega^{-1}x) = o(1) \quad in \quad & S_1 := \{z \in \mathbb{C} / -\frac{\pi}{3} \leq |\arg(z)| \leq \pi\}; \\ Ai(x) = o(1) \quad in \quad & S_0 := \{z \in \mathbb{C} / -\frac{\pi}{3} \leq |\arg(z)| \leq \frac{\pi}{3}\}. \end{aligned} \tag{3.6.7}$$

The computation of Wronskian determinants leads to:

$$\begin{aligned} W\{Ai(x), Bi(x))\} &= \frac{1}{\pi}; \\ W\left\{Ai(\omega x), Ai(\omega^{-1}x)\right\} &= \frac{1}{2\pi i}; \\ W\left\{Ai(x), Ai(\omega^{\mp 1}x)\right\} &= \frac{e^{\pm i\pi/6}}{2\pi}. \end{aligned} \tag{3.6.8}$$

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