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# Semi-classical analysis

Clotilde Fermanian Kammerer & Jérôme Le Rousseau

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## 1 Introduction

### 1.1 What is semi-classical analysis ?

Semi-classical analysis has its roots in the foundations of quantum mechanics. Simultaneously with this new theory arose the question of understanding the links between classical and quantum mechanics. It turned out that the Planck constant  $\hbar$  can be understood as the obstruction to give a classical description of a quantum particle by the simultaneous knowledge of its position and its momentum. This is expressed by the Heisenberg uncertainty principle that we first discuss.

In quantum mechanics, a particle is described by a probability measure  $|\psi(x)|^2 dx$ , with  $\psi$  a normalized square integrable function on the configuration space  $\mathbb{R}_x^d$ , called its wave function. Denoting by  $x_j$  the coordinates of  $x \in \mathbb{R}^d$ , the average position of the particle is

$$\langle x_j \rangle_\psi = \int_{\mathbb{R}^d} x_j |\psi(x)|^2 dx, \quad 1 \leq j \leq d,$$

that is, the expectation value of the observable  $x_j$ . Similarly, the average momentum is

$$\langle \xi_j \rangle_\psi = \int_{\mathbb{R}^d} \hbar D_{x_j} \psi(x) \bar{\psi}(x) dx, \quad D_{x_j} = \frac{1}{i} \partial_{x_j}. \quad (1)$$

Considering the variance of these random variables,

$$\begin{aligned} (d_\psi x_j)^2 &= \langle (x_j - \langle x_j \rangle_\psi)^2 \rangle_\psi, \\ (d_\psi \xi_j)^2 &= \langle (\xi_j - \langle \xi_j \rangle_\psi)^2 \rangle_\psi, \end{aligned}$$

the Heisenberg uncertainty principle reads

$$d_\psi x_j d_\psi \xi_j \geq \frac{\hbar}{2}, \quad 1 \leq j \leq d.$$

It relies on the Cauchy-Schwarz inequality

$$\begin{aligned} &|\operatorname{Im} \langle (x_j - \langle x_j \rangle_\psi) \psi, (\hbar D_{x_j} - \langle \xi_j \rangle_\psi) \psi \rangle_{L^2}| \\ &\leq \| (x_j - \langle x_j \rangle_\psi) \psi \|_{L^2} \| (\hbar D_{x_j} - \langle \xi_j \rangle_\psi) \psi \|_{L^2} \\ &= d_\psi x_j d_\psi \xi_j, \end{aligned}$$

and the observation

$$\begin{aligned} &\operatorname{Im} \langle (x_j - \langle x_j \rangle_\psi) \psi, (\hbar D_{x_j} - \langle \xi_j \rangle_\psi) \psi \rangle_{L^2} \\ &= \frac{1}{2i} \langle [\hbar D_{x_j} - \langle \xi_j \rangle_\psi, x_j - \langle x_j \rangle_\psi] \psi, \psi \rangle_{L^2} = -\frac{\hbar}{2}. \end{aligned}$$

The Planck constant  $\hbar$  reflects the difference between quantum and classical mechanics, since, in the latter, the position and the momentum are deterministic variables. The subject of semi-classical analysis is to understand how one can derive classical mechanics from quantum mechanics. Even though  $\hbar$  is a physical constant, this is done by performing the limit  $\hbar \rightarrow 0$ . For this reason, we will skip the notation  $\hbar$  and denote by  $h$  a small parameter that is present in some problems of interest involving PDEs. Carrying a semi-classical analysis of this problem consists in investigating the properties of a phenomenon of interest in the limit  $h \rightarrow 0$ . This type of analysis led to the development of asymptotic technics that are now used in various fields of applied mathematics. Examples are the determination of the asymptotics of the spectrum of Schrödinger operators or the characterization of the properties of the solutions to time-dependent Schrödinger equations.

### 1.2 Outline

We introduce in Section 2 three representative topics in semi-classical analysis. Starting from the correspondence between classical and quantum mechanics, basic semi-classical analysis tools and results are presented in Section 3. In Section 4, the three problems of Section 2 are investigated in the light of the introduced techniques allowing one to emphasize different aspects of semi-classical analysis.

## 2 Some semi-classical problems

Three problems are presented. They originate from various fields: theoretical chemistry, spectral geometry, and control theory. In each case the semi-classical parameter has a different interpretation.

### 2.1 Schrödinger equation in the Born-Oppenheimer approximation

The dynamics of a molecule consisting in  $k_e$  electrons and  $k_n$  nuclei of masses  $(M_j)_{1 \leq j \leq k_n}$  (in atomic units) is described by a wave function belonging

to  $L^2(\mathbb{R}^{3k_e+3k_n})$ . Dating from the 30s, the *Born-Oppenheimer approximation* [10] suggests to take advantage of the fact that,  $m_e$  being the mass of an electron, the ratio  $m_e/M_j$  is small, for all the nuclei, and roughly, of the main size, even though the  $j$ -th atoms are different. Setting

$$\sqrt{\frac{m_e}{M_j}} \sim h, \quad 1 \leq j \leq k_n,$$

one introduces in the equations the small parameter  $h$  and writes

$$\widehat{H}_{\text{mol}} = -\frac{h^2}{2}\Delta_x + \widehat{H}_e(x),$$

where  $x$  is in  $\mathbb{R}^{3k_n}$  and denotes the coordinates of the nuclei and the electronic Hamiltonian  $\widehat{H}_e(x)$  takes into account the kinetics of the electrons, together with the interactions between the electrons themselves, nuclei, and electron/nuclei.

For all  $x$  in  $\mathbb{R}^{3k_n}$ , the operator  $\widehat{H}_e(x)$  is a self-adjoint operator on  $L^2(\mathbb{R}^{3k_e})$  with spectrum  $\sigma_e(x)$  that depends on the configuration  $x$  of the nuclei. When the initial data  $\psi_0^h$  is in the vector-sum of  $N$  eigenspaces of  $H_e(x)$  corresponding to  $N$  eigenvalues isolated from the remainder of the spectrum, it has been proved in [83, 71], that, considering semi-classical times  $t \sim \frac{1}{h}$ , one is left with a system of semi-classical Schrödinger equations

$$ih\partial_t\psi^h = -\frac{h^2}{2}\Delta\psi^h + V(x)\psi^h, \quad (t, x) \in \mathbb{R} \times \mathbb{R}^d, \quad (2)$$

with  $\psi^h \in L^2(\mathbb{R}^d, \mathbb{C}^N)$  and  $V$  a smooth matrix-valued potential. The analysis is thus reduced to a finite number of spectral components, and, as discussed in Section 4.1, semi-classical technics allow one to develop numerical tools adapted for solving these equations [60].

## 2.2 Eigenfunctions of the Laplacian and quantum limits

Let us consider  $(M, g)$  a smooth compact Riemannian manifold without boundary. The Laplace-Beltrami operator  $-\Delta_M$  is a nonnegative self-adjoint operator with compact resolvent, and admits a sequence of normalized eigenfunctions  $(\varphi_k)_{k \in \mathbb{N}}$  and eigenvalues  $(E_k)_{k \in \mathbb{N}}$ , ordered in increasing order:

$$\begin{aligned} -\Delta_M \varphi_k &= E_k \varphi_k, \\ 0 &= E_1 \leq E_2 \leq \dots \leq E_k \leq \dots, \quad E_k \xrightarrow[k \rightarrow \infty]{} +\infty. \end{aligned} \quad (3)$$

A historical question [28] concerns the densities

$$\nu_k(x) = |\varphi_k(x)|^2 dx,$$

and the analysis of their limit points, measures on  $M$ , as  $k \rightarrow +\infty$ . Such measures are called *quantum limits*. Setting

$$h_k = \frac{1}{\sqrt{E_k}},$$

one is left with a semi-classical problem consisting in the analysis of a sequence of wave functions  $(\varphi_k)_{k \in \mathbb{N}}$  satisfying the semi-classical PDE

$$-h_k^2 \Delta_M \varphi_k = \varphi_k.$$

As we shall see in Section 4.2, this approach of the problem allows one to derive fundamental properties of the quantum limits, leading in certain cases, to their determination (see the *Schnirelman Theorem* and its proofs by Y. Colin de Verdière and S. Zelditch, independently, [86, 20, 91], or the surveys [4, 3]).

This type of question is also posed in the context of random surfaces with genus that tends to infinity, the semi-classical parameter is then the inverse of the genus [75]. These examples and the preceding one illustrate that the physical meaning of the semi-classical parameter may be far from the actual Planck constant  $\hbar$ .

In the preceding two examples, the small scale  $h$  appears naturally and its presence in the equations endows the solutions with specific features. For example, the family of eigenfunctions  $(\varphi_k)_{k \in \mathbb{N}}$  in (3) have  $H^s$ -Sobolev norms of size  $h_k^{-s}$ . One can also argue in the converse sense and, given a family of square-integrable functions, analyze its oscillations at some precise scale that we fix, e.g.  $h = 2^{-n}$  for  $n \in \mathbb{N}$ . As illustrated in the next section, this strategy can be used to prove that solutions to dispersive evolution equations such as wave-type equations or the Schrödinger equation are observable.

## 2.3 High-frequency analysis and control theory

On a compact Riemannian manifold  $(M, g)$  without boundary, consider the following free wave equation, here of Klein-Gordon type,

$$\partial_t^2 u - \Delta_M u + u = 0, \quad (u, \partial_t u)|_{t=0} = (u_0, u_1). \quad (4)$$

It is well-posed for  $(u_0, u_1) \in H^1(M) \times L^2(M)$ . Given an open subset  $\omega$  of  $M$  and  $T > 0$ , one says that the wave equation is observable from  $\omega$  in time  $T > 0$  if there exists  $C > 0$  such that

$$\mathcal{E}(u) \leq C \int_0^T \|1_\omega \partial_t u\|_{L^2(M)}^2 dt, \quad (5)$$

for any solution  $u$  to (4), where  $\mathcal{E}(u)$  denotes the energy of the solution

$$\mathcal{E}(u) = \frac{1}{2} (\|u_0\|_{H^1(M)}^2 + \|u_1\|_{L^2(M)}^2).$$

With a duality argument [67], an observability inequality as in (5) is equivalent to the exact controllability of the wave equation from  $\omega$  in time  $T$ , that is, for any initial and final states,  $(y_0, y_1)$  and  $(y_0^T, y_1^T)$  both in  $H^1(M) \times L^2(M)$ , the ability to find  $f \in L^2((0, T) \times M)$  such that the solution  $y$  to

$$\partial_t^2 y - \Delta_M y + y = 1_\omega f, \quad (y, \partial_t y)|_{t=0} = (y_0, y_1),$$

satisfies  $(y, \partial_t y)|_{t=T} = (y_0^T, y_1^T)$ .

As shown in [64, 13], for the proof of (5) it suffices to consider sequences of waves  $(u_k)_{k \in \mathbb{N}}$  with localized time-frequency  $\tau \sim h^{-1} \sim 2^n$ ,  $n \in \mathbb{N}$ , built by means of the eigenfunctions  $\varphi_k$  defined in (3), with  $\sqrt{E_k} \sim h^{-1}$ . Although not intrinsic to the considered question, Section 4.3 discusses how a semi-classical point of view can be chosen, offering a powerful analysis toolbox.

### 3 Correspondence principle

The phase space of quantum mechanics is the set  $\mathbb{R}^{2d}$  of positions and momenta:

$$z = (x, \xi) \in \mathbb{R}^{2d}.$$

The Fourier transform  $f \mapsto \widehat{f}$  is given by

$$\widehat{f}(\xi) = \int_{\mathbb{R}^d} f(x) e^{-ix \cdot \xi} dx, \quad \xi \in \mathbb{R}^d,$$

and  $f \mapsto \mathcal{F}(f) = (2\pi)^{-\frac{d}{2}} \widehat{f}$  is a unitary transformation of  $L^2(\mathbb{R}^d)$ . In a semi-classical context, one rescales the Fourier transform by considering the  $h$ -Fourier transform  $f \mapsto \mathcal{F}_h f$

$$\mathcal{F}_h f(\xi) = (2\pi h)^{-\frac{d}{2}} \widehat{f}\left(\frac{\xi}{h}\right), \quad \xi \in \mathbb{R}^d.$$

Note that by the Plancherel theorem, the average momentum introduced in (1) reads

$$\langle \xi_j \rangle_\psi = \int_{\mathbb{R}^d} \xi_j |\mathcal{F}_h \psi(\xi)|^2 d\xi.$$

The phase space  $\mathbb{R}^d \times \mathbb{R}^d$  is endowed with the symplectic form  $\omega = d\xi \wedge dx$  defined by

$$\omega(z, z') = Jz \cdot z', \quad J = \begin{pmatrix} 0 & \text{Id}_d \\ -\text{Id}_d & 0 \end{pmatrix}, \quad z, z' \in \mathbb{R}^{2d}. \quad (6)$$

Geometrically, it is natural to view the phase space as the cotangent bundle  $T^*\mathbb{R}^d$ , with  $\xi \in T_x^*\mathbb{R}^d$ , the cotangent variable (see Section 4.2).

### 3.1 Semi-classical wave packets

Semi-classical wave packets are wave functions associated with a classical state  $z = (q, p) \in \mathbb{R}^{2d}$ . One defines Gaussian wave packets as

$$g_z^h(x) = (\pi h)^{-d/4} \exp\left(-\frac{1}{2h}|x - q|^2 + \frac{i}{h}p \cdot (x - q)\right),$$

for  $x \in \mathbb{R}^d$ . It is normalized,  $\|g_z^h\|_{L^2} = 1$ , and centered in  $z$ ,

$$\langle x_j \rangle_{g_z^h} = q_j \quad \text{and} \quad \langle \xi_j \rangle_{g_z^h} = p_j, \quad 1 \leq j \leq d.$$

Moreover, its  $h$ -Fourier transform has the same structure

$$\mathcal{F}_h \left( e^{i\frac{p \cdot q}{2h}} g_z^h \right) = e^{i\frac{p \cdot (-q)}{2h}} g_{jz}^h, \quad z = (q, p) \in \mathbb{R}^{2d}.$$

The Gaussian wave packets were introduced in part because they have the unique property among  $L^2$ -functions of saturating the uncertainty principle

$$d_{g_z^h} x_j = d_{g_z^h} \xi_j = \sqrt{\frac{h}{2}}, \quad 1 \leq j \leq d.$$

Besides, any wave function can be written as a superposition of Gaussian wave packets according to the Bargmann formula: for all  $f \in L^2(\mathbb{R}^d)$

$$f = (2\pi h)^{-\frac{d}{2}} \int_{\mathbb{R}^{2d}} \mathcal{B}_h[f](z) g_z^h dz, \quad (7)$$

where the Bargmann transform [23] is the isometry from  $L^2(\mathbb{R}^d)$  into  $L^2(\mathbb{R}^{2d})$  defined by

$$\mathcal{B}_h[f](z) = (2\pi h)^{-\frac{d}{2}} (f, g_z^h)_{L^2}, \quad z \in \mathbb{R}^{2d}.$$

### 3.2 Semi-classical pseudodifferential operators and related notions

A question that arises from quantum mechanics is the quantization problem, or how to associate an operator to an energy, also called Hamiltonian. It gives a mathematical setting to explore the correspondence between classical and quantum mechanics.

#### 3.2.1 Quantization of observables

Let  $a(x, \xi)$  be a semi-classical observable in the Schwartz space  $\mathcal{S}(\mathbb{R}^{2d})$ . The *semi-classical pseudodifferential operator* ( $h$ - $\psi$ do), of symbol  $a$  is the operator  $\text{Op}_h(a)$  defined on functions  $f \in \mathcal{S}(\mathbb{R}^d)$  by

$$\begin{aligned} \text{Op}_h(a)f(x) &= (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} a\left(\frac{1}{2}(x+y), \xi\right) e^{\frac{i}{h}\xi \cdot (x-y)} f(y) dy d\xi. \end{aligned}$$

This form is called the *Weyl-quantization* of the symbol  $a$  [54, 25, 70, 93].

The operator  $\text{Op}_h(a)$  maps  $\mathcal{S}(\mathbb{R}^d)$  into itself and, by duality,  $\mathcal{S}'(\mathbb{R}^d)$  into itself. Its kernel  $k_h$  can be expressed in terms of the inverse Fourier transform of  $a$  in the variable  $\xi$

$$\kappa(x, v) = (2\pi)^{-d} \int_{\mathbb{R}^d} a(x, \xi) e^{i\xi \cdot v} d\xi, \quad (x, v) \in \mathbb{R}^{2d}. \quad (8)$$

Indeed, one has

$$k_h(x, y) = \frac{1}{h^d} \kappa\left(\frac{x+y}{2}, \frac{x-y}{h}\right), \quad (x, y) \in \mathbb{R}^{2d}.$$

As a consequence of the Schur Lemma, the operator  $\text{Op}_h(a)$  maps  $L^2(\mathbb{R}^d)$  into itself and

$$\begin{aligned} \|\text{Op}_h(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} &\leq \int_{\mathbb{R}^d} \sup_{x \in \mathbb{R}^d} |\kappa(x, v)| dv \\ &\leq C \sup_{\substack{\beta \in \mathbb{N}^d \\ |\beta| \leq d+1}} \sup_{x \in \mathbb{R}^d} \|\partial_\xi^\beta a(x, \cdot)\|_{L^1(\mathbb{R}^d)}, \end{aligned}$$

for  $C > 0$  independent of  $a$  and  $h$ . The Calderón-Vaillancourt theorem [17, 56, 23] also gives the existence of  $C > 0$  such that for all  $a$  and  $h$ ,

$$\begin{aligned} \|\text{Op}_h(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} &\leq C \sum_{\alpha \in \mathbb{N}^{2d}, |\alpha| \leq 2d+1} h^{\frac{|\alpha|}{2}} \sup_{\mathbb{R}^d \times \mathbb{R}^d} |\partial_{x, \xi}^\alpha a|. \end{aligned}$$

This estimate can be derived from the case  $h = 1$  by conjugating  $\text{Op}_h(a)$  by the scaling unitary operator  $T_h : f \mapsto h^{\frac{d}{4}} f(\sqrt{h} \cdot)$ . Indeed, one has  $T_h \text{Op}_h(a) T_h^* = \text{Op}_1(a(\sqrt{h} \cdot, \sqrt{h} \cdot))$ .

The present definition of  $h$ - $\psi$ dos can be set within the general Hörmander formalism with the phase space metric  $|dx|^2 + h^2|d\xi|^2$ ; see [55, Sections 18.4-5], [65, Section 2] and [70, Sections 2.2-2.3].

### 3.2.2 Symbolic calculus

The set of  $h$ - $\psi$ dos is an algebra that enjoys symbolic calculus. If  $a, b \in \mathcal{S}(\mathbb{R}^{2d})$ , then in  $\mathcal{L}(L^2(\mathbb{R}^d))$ ,

$$\begin{aligned} \text{Op}_h(a) \text{Op}_h(b) &= \text{Op}_h(ab) \\ &+ \frac{h}{2i} \text{Op}_h(\{a, b\}) + O(h^2), \end{aligned} \quad (9)$$

where  $\{a, b\}$  denotes the *Poisson bracket*

$$\{a, b\} = \nabla_\xi a \cdot \nabla_x b - \nabla_x a \cdot \nabla_\xi b.$$

This implies that the commutator of two  $h$ - $\psi$ dos is of lower order, which turns out to read

$$[\text{Op}_h(a), \text{Op}_h(b)] = \frac{h}{i} \text{Op}_h(\{a, b\}) + O(h^3), \quad (10)$$

because of the symmetries of the term  $O(h^2)$  in (9).

The remainder terms  $O(h^2)$ ,  $O(h^3)$  appearing in (9) and (10), involve Schwartz semi-norms of the symbols  $a$  and  $b$ , such as

$$N_k(a) = \sup_{|\gamma| \leq k} \|\partial_z^\gamma a\|_{L^\infty}.$$

for  $k \in \mathbb{N}$  large enough [79].

Regarding the adjoint, one simply has

$$\text{Op}_h(a)^* = \text{Op}_h(\bar{a}). \quad (11)$$

In particular, if  $a$  is real-valued, then  $\text{Op}_h(a)$  is a symmetric bounded operator, thus self-adjoint. Results of this section can be found in [25, 93, 4], for example.

Other quantizations also enjoy a symbolic calculus. Let us cite the *left-quantization* [73], so-called *classical quantization*,  $a \mapsto a(x, hD)$  defined by

$$\begin{aligned} a(x, hD)f(x) &= (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} a(x, \xi) e^{\frac{i}{h}\xi \cdot (x-y)} f(y) dy d\xi \\ &= (2\pi)^{-d} \int_{\mathbb{R}^d} a(x, h\xi) e^{i\xi \cdot x} \widehat{f}(\xi) d\xi, \quad f \in \mathcal{S}(\mathbb{R}^d). \end{aligned}$$

However, the symbol for the adjoint operator is not as simple as in (11) and the remainder in the counterpart to (10) is only  $O(h^2)$  in the left-calculus. This is a reason for the Weyl-quantization to be often preferred. Correspondance between the two quantizations is expressed by

$$a(x, \xi) = e^{\frac{i\hbar}{2} D_x \cdot D_\xi} b(x, \xi),$$

if  $a(x, hD) = \text{Op}_h(b)$ , [25].

The notations  $a(x, hD)$  and  $\text{Op}_h(a)$  are extended to smooth functions  $(x, \xi) \mapsto a(x, \xi)$  that satisfy symbol estimates of the form

$$\forall \alpha, \beta \in \mathbb{N}^d, \exists C_{\alpha, \beta} > 0, \left\| \langle \xi \rangle^{-m+|\beta|} \partial_x^\alpha \partial_\xi^\beta a \right\|_{L^\infty} \leq C_{\alpha, \beta}$$

for some  $m \in \mathbb{N}$  (here  $\langle \xi \rangle = \sqrt{1 + |\xi|^2}$ ). One then says that  $a \in S^m$  [93].

In particular, this class contains the functions  $p$  that are polynomial functions of degree  $m$  in the variable  $\xi$  with coefficients that are smooth bounded functions of  $x$  with bounded derivatives. In this case, the operators  $p(x, hD)$  and  $\text{Op}_h(p)$  are differential operators.

For such symbol classes, symbolic calculus results above also hold. In particular, if  $a \in S^m$  and  $b \in S^{m'}$ , then  $\text{Op}_h(a) \text{Op}_h(b) = \text{Op}_h(c)$  with  $c \in S^{m+m'}$  given by  $c = ab + h\{a, b\}/(2i) \bmod h^2 S^{m+m'-2}$ .

Introducing the semi-classical Sobolev norms

$$\|f\|_s = \sup_{0 \leq \ell \leq s} \|\langle hD_x \rangle^\ell f\|_{L^2}, \quad s \in \mathbb{R},$$

if  $a \in S^m$  and  $s \in \mathbb{R}$ , there exists a constant  $C > 0$  such that

$$\|\text{Op}_h(a)f\|_s \leq C \|f\|_{s+m}, \quad h \in (0, 1], \quad f \in \mathcal{S}(\mathbb{R}^d).$$

### 3.2.3 Bargmann transform and $h$ - $\psi$ dos

The relations of  $h$ - $\psi$ dos with the Bargmann transform enlighten the role of the  $h$ - $\psi$ dos in terms of microlocalization. For  $a \in \mathcal{S}(\mathbb{R}^{2d})$ , there exists a constant  $C > 0$  such that for  $h \in (0, 1]$ ,

$$\|\mathrm{Op}_h(a) - \mathcal{B}_h^* a \mathcal{B}_h\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq Ch. \quad (12)$$

Indeed, the kernel of the operator  $\mathcal{B}_h^* a \mathcal{B}_h$  is the function

$$\kappa_h^{\mathcal{B}}(x, y) = \frac{1}{h^d} \kappa_h^{\mathcal{B}}\left(\frac{x+y}{2}, \frac{x-y}{h}\right), \quad (x, y) \in \mathbb{R}^{2d},$$

related with the function  $\kappa$  of (8) according to

$$\kappa_h^{\mathcal{B}}(x, v) = \pi^{-\frac{d}{2}} e^{-\frac{h}{4}|v|^2} \int_{\mathbb{R}^d} \kappa(x - \sqrt{h}q, v) e^{-|q|^2} dq,$$

for  $(x, v) \in \mathbb{R}^{2d}$ . Therefore, using Taylor expansions, the fact that  $\int q e^{-|q|^2} = 0$ , and the rapid decay of  $\kappa(x, v)$  in  $v$  one obtains

$$\kappa_h^{\mathcal{B}}(x, v) - \kappa(x, v) = h \int_{\mathbb{R}^d} A_h(x, q, v) e^{-|q|^2} dq,$$

where for all  $N \in \mathbb{N}$ , the function

$$(x, q, v) \mapsto |v|^N A_h(x, q, v)$$

is uniformly bounded in  $h \in (0, 1]$ . Estimate (12) then comes from the Schur Lemma.

### 3.2.4 Ellipticity, parametrix, and sharp Gårding inequality

Symbolic calculus allows one to transfer properties of the symbol  $a$  to the  $h$ - $\psi$ do  $\mathrm{Op}_h(a)$ .

Let  $P^h = p(x, hD)$  be a differential operator with a symbol  $p(x, \xi)$  that is a smooth polynomial function of degree  $m$  in  $\xi$

$$p(x, \xi) = \sum_{|\alpha| \leq m} p_\alpha(x) \xi^\alpha.$$

One has  $p \in S^m$ . The symbol  $p$  is said to be *elliptic* if there exists  $C > 0$  and  $R > 0$  such that

$$|p(x, \xi)| \geq C |\xi|^m, \quad (x, \xi) \in \mathbb{R}^{2d}, \quad |\xi| \geq R.$$

In such a case, the  $h$ - $\psi$ do  $P^h$  is one to one from  $H_h^{s+m}(\mathbb{R}^d)$  onto  $H_h^s(\mathbb{R}^d)$  for all  $s \in \mathbb{R}$  and

$$(P^h)^{-1} = \mathrm{Op}_h(p^{-1}) + O(h),$$

by symbolic calculus. One has  $p^{-1} \in S^{-m}$  and  $\mathrm{Op}_h(p^{-1})$  is called a *parametrix* of  $P^h$ .

The question of positivity is addressed by the sharp *Gårding inequality*, which is a direct consequence of estimate (12). There exist  $C, N > 0$  such that for all  $a$  in  $\mathcal{S}(\mathbb{R}^d)$  satisfying  $a \geq 0$ , we have for all  $f$  in  $\mathcal{S}(\mathbb{R}^d)$  and  $h$  in  $(0, 1]$ .

$$(f, \mathrm{Op}_h(a)f) \geq -Ch \|f\|_{L^2} \sup_{|\alpha| \leq N} \|\partial_z^\alpha a\|_{L^\infty}. \quad (13)$$

### 3.2.5 Functional calculus and trace formula

Since  $\mathrm{Op}_h(a)$  is a bounded self-adjoint operator for real-valued  $a$  in  $\mathcal{S}(\mathbb{R}^d)$ , functional calculus can be used and the operator  $F(\mathrm{Op}_h(a))$  is well defined for  $F$  continuous on  $\mathbb{R}$ .

Suppose  $F \in \mathcal{C}_c^\infty(\mathbb{R})$ . Then,  $F(\mathrm{Op}_h(a))$  coincides asymptotically with a pseudodifferential operator of symbol  $F(a)$ , that is,

$$F(\mathrm{Op}_h(a)) = \mathrm{Op}_h(F(a)) + O(h) \quad \text{in } \mathcal{L}(L^2(\mathbb{R}^d)). \quad (14)$$

This relies on the *Helffer-Sjöstrand formula* [93, 25] that plays an important role in semi-classical analysis and is of interest in itself, in particular because of the alternative construction of the functional calculus it provides for a (possibly unbounded) self-adjoint operator [24].

In fact, for all  $n \in \mathbb{N}$ ,  $F$  has an almost analytic continuation, that is, a function  $\tilde{F}_n \in \mathcal{C}_c^\infty(\mathbb{C})$  that coincides with  $F$  on  $\mathbb{R}$  and such that

$$\left| \bar{\partial} \tilde{F}_n(z) \right| \leq C |\mathrm{Im}(z)|^n, \quad z \in \mathbb{C}. \quad (15)$$

The Helffer-Sjöstrand formula reads

$$F(\mathrm{Op}_h(a)) = \frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{F}_n(z) (\mathrm{Op}_h(a) - z)^{-1} L(dz),$$

where  $L(dz)$  is the Lebesgue measure on  $\mathbb{C}$ . The operator  $(\mathrm{Op}_h(a) - z)^{-1}$  is bounded, with norm  $|\mathrm{Im}(z)|^{-1}$  for almost all  $z \in \mathbb{C}$  and, thanks to (15), using a parametrix of  $\mathrm{Op}_h(a) - z$  to replace the resolvent  $(\mathrm{Op}_h(a) - z)^{-1}$  one obtains (14).

Noticing that for all fixed  $h > 0$ ,  $\mathrm{Op}_h(a)$  is a compact operator with Hilbert-Schmidt norm

$$\|\mathrm{Op}_h(a)\|_{\mathrm{HS}(L^2(\mathbb{R}^d))} = (2\pi h)^{-d/2} \|a\|_{L^2(\mathbb{R}^{2d})},$$

one deduces a trace formula: for  $F \in \mathcal{C}_c^\infty(\mathbb{R})$  nonnegative one has

$$\mathrm{Tr}(F(\mathrm{Op}_h(a))) \quad (16)$$

$$\underset{h \rightarrow 0}{\sim} (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} F(a(x, \xi)) dx d\xi.$$

This approach is used in the spectral analysis of Schrödinger operators such as  $-h^2 \Delta + V(x)$  for confining potential, or magnetic Schrödinger operators  $-|hD_x - A(x)|^2$  on bounded domains (see the historical series of papers by B. Helffer and J. Sjöstrand [48, 49, 50, 51] and the books [34, 78, 85]).

### 3.3 Wigner transform and semi-classical measures

#### 3.3.1 Main definitions and example

Following E. Wigner [90], once given a bounded family  $(\psi^h)_{h>0}$  in  $L^2(\mathbb{R}^d)$ , one can consider the distribution

$$W[\psi^h] : a \mapsto \langle W[\psi^h], a \rangle = (\text{Op}_h(a)\psi^h, \psi^h)$$

called the *Wigner transform* of  $(\psi^h)_{h>0}$ . One finds it is defined for  $(x, \xi) \in \mathbb{R}^{2d}$  by

$$W[\psi^h](x, \xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{iv \cdot \xi} \times \psi^h \left( x - \frac{h}{2}v \right) \overline{\psi^h} \left( x + \frac{h}{2}v \right) dv. \quad (17)$$

This notion has been revisited in the 1990's, see [46, 68] and the works of P. Gérard and his coauthors [37, 39, 40].

In view of (13), for any family, weak limits point in the sense of distributions of the Wigner transform of  $(\psi^h)_{h>0}$  are finite nonnegative measures. They are called *semi-classical measures* of the family  $(\psi^h)_{h>0}$  (see [46, 37, 39]). One also uses the term *Wigner measures* (see [40]). For such a measure  $\mu$ , there exists a subsequence  $h_k \rightarrow 0$  such that

$$\langle W[\psi^{h_k}], a \rangle \rightarrow \langle \mu, a \rangle, \quad \forall a \in \mathcal{C}_c^\infty(\mathbb{R}^{2d}). \quad (18)$$

For example, the Wigner transform of the Gaussian wave packet  $g_z^h$  is given for  $z, \zeta \in \mathbb{R}^{2d}$  by

$$W[g_z^h](\zeta) = (\pi h)^{-d} \exp(-\frac{1}{h}|\zeta - z|^2).$$

Thus, the family  $(g_z^h)_{h>0}$  has only one semi-classical measure, namely,

$$\mu(x, \xi) = \delta(x - q) \otimes \delta(\xi - p).$$

In the limit  $h \rightarrow 0$ , the wave function  $g_z^h$  converges to the classical state  $z = (q, p)$ , which gives a first illustration of the correspondence principle.

#### 3.3.2 $h$ -oscillation

There is a connexion between the weak limits of  $|\psi^h(x)|^2 dx$  and the semi-classical measures of  $(\psi^h)_{h>0}$ . Indeed, if the sequence  $(h_k)_{k \in \mathbb{N}}$  and the measure  $\mu$  fulfills property (18) and if  $\nu$  is a weak limit of the measure  $|\psi^{h_k}(x)|^2 dx$ , then

$$\nu(\{x\}) \geq \mu(\{x\} \times \mathbb{R}^d)$$

as measures on  $\mathbb{R}_x^d$ . Besides, equality holds if  $(\psi^h)_{h>0}$  is  $h$ -oscillating, namely satisfies the property

$$\limsup_{h \rightarrow 0} \int_{h|\xi| \geq R} |\widehat{\psi^h}(\xi)|^2 d\xi \xrightarrow{R \rightarrow +\infty} 0.$$

In other words, no mass escapes to infinity in frequency. Such a property is satisfied for examples if  $(\langle hD_x \rangle^s \psi^h)_{h>0}$  is uniformly bounded in  $L^2(\mathbb{R}^d)$  for some  $s > 0$ . In fact, once given a bounded family in  $L^2(\mathbb{R}^d)$ , an appropriate semi-classical scale (if any) can be sought by analyzing the size of one of its Sobolev norms, motivating a semi-classical analysis at that precise scale. Such strategies will be implemented in Sections 4 for the analysis of the examples presented in Section 2.

#### 3.3.3 Wave front set

The support of the semi-classical measure of a bounded family  $(\psi^h)_{h>0}$  in  $L^2(\mathbb{R}^d)$  is included in the *semi-classical wave front set* denoted  $\text{WF}_h(\psi^h)$ . The latter is characterized by the following property:  $(x, \xi) \notin \text{WF}_h(\psi^h)$  if and only if there exists an open neighborhood  $U$  of the point  $(x, \xi)$  and a function  $a \in \mathcal{C}_c^\infty(U)$  such that

$$a(x, \xi) \neq 0$$

$$\text{and } \forall n \in \mathbb{N}, \quad \|\text{Op}_h(a)\psi^h\|_{L^2} = O(h^n).$$

If  $\mu$  is a semi-classical measure of  $(\psi^h)_{h>0}$  for the scale  $h_k$ ,

$$\text{Supp } \mu \subset \text{WF}_{h_k}(\psi^{h_k}).$$

Historically, the semi-classical wave front set was introduced earlier than semi-classical measures. It is closely related to microlocal versions of wave front set where no scale is emphasized (see [53, Vol. 1, Ch. 8]).

#### 3.3.4 Semi-classical measures and PDEs

Consider  $P^h = p(x, hD)$  a differential operator. Suppose  $(\psi^h)_{h>0}$  is a sequence of bounded  $L^2$ -functions associated with a semi-classical measure  $\mu$  such that

$$P^h \psi^h = o(1)$$

in  $L^2(\mathbb{R}^d)$  as  $h \rightarrow 0$ . Then, for  $a \in \mathcal{S}(\mathbb{R}^{2d})$ ,

$$(\text{Op}_h(a)P^h \psi^h, \psi^h)_{L^2} = o(1),$$

implying  $\langle \mu, ap \rangle = 0$  and

$$\text{supp}(\mu) \subset \text{Char}(P^h), \quad (19)$$

where  $\text{Char}(P^h) = \{p(x, \xi) = 0\}$  is the *characteristic set* of  $p$ .

Assume moreover that  $P^h$  is symmetric and

$$P^h \psi^h = o(h)$$

in  $L^2(\mathbb{R}^d)$  as  $h \rightarrow 0$ . Then, for  $a \in \mathcal{S}(\mathbb{R}^{2d})$ ,

$$([\text{Op}_h(a), P^h] \psi^h, \psi^h)_{L^2} = o(h),$$

implying  $\langle \mu, \{p, a\} \rangle = 0$ . One has  $\{p, a\} = H_p a$  with  $H_p = J \nabla_{x, \xi} p$ , the Hamiltonian vector field associated with  $p$  (recall that  $J$  is given by (6)). Since  ${}^t H_p = -H_p$  one finds

$$H_p \mu = 0, \quad (20)$$

in the sense of distributions, meaning with (19) that  $\mu$  is invariant along the Hamiltonian curves  $(\Phi^t(z))_{t \in \mathbb{R}}$  for  $z \in \mathbb{R}^{2d}$  where the map  $\Phi^t : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ , is determined by

$$\dot{\Phi}^t = H_p(\Phi^t), \quad \Phi^0 = \text{Id}_{\mathbb{R}^{2d}}. \quad (21)$$

For all  $t \in \mathbb{R}$ ,  $z \mapsto \Phi^t(z)$  is a symplectomorphism (it preserves the symplectic form  $\omega$  given in (6)). Condition (20) relates classical phase-space trajectories and solutions concentrations.

Propagation of semi-classical measures is more difficult to prove if coefficients are singular. We refer for instance to [36, 35, 14].

### 3.4 Semi-classical evolution

Consider an evolution equation involving a smooth time-dependent Hamiltonian function  $p : \mathbb{R} \times \mathbb{R}^{2d} \rightarrow \mathbb{R}$ , with sub-quadratic growth

$$\forall N \geq 2, \exists C_N > 0, \sup_{|\beta|=N} \sup_{(t,z) \in \mathbb{R} \times \mathbb{R}^{2d}} \left| \partial_z^\beta p(t, z) \right| \leq C_N.$$

Then, the operator  $P^h(t) = \text{Op}_h(p(t))$  is self-adjoint and there exists a strongly continuous two-parameters family of unitary operators  $U^h(t, s)$  such that

$$ih \frac{d}{dt} U^h(t, s) = P^h(t) U^h(t, s), \quad U^h(s, s) = \text{Id}_{L^2}$$

on the domain of the operator  $P^h(t)$  (see [77]). If  $P^h$  is independent of time, then  $U^h(t, s) = U^h(t - s, 0)$ , and  $U^h(t, 0)$  is the semigroup generated by  $P^h$ .

#### 3.4.1 The Egorov Theorem

At the classical level, one associates with  $p(t)$  the ordinary differential system  $\partial_t z = H_{p(t)}(t, z)$  and the flow map  $\Phi^{t,s} : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ , that is determined by

$$\partial_t \Phi^{t,s} = H_{p(t)}(t, \Phi^{t,s}), \quad \Phi^{s,s} = \text{Id}_{\mathbb{R}^{2d}}. \quad (22)$$

Note that if  $p = p(z)$  does not depend on the time,  $\Phi^{t,s} = \Phi^{t-s}$  defined in (21).

For the evolution of an observable  $a \in \mathcal{S}(\mathbb{R}^{2d})$  one uses the Liouvillian  $\mathcal{L}_{t,s} a = a \circ \Phi^{t,s}$  that satisfies the transport equation

$$\partial_t (\mathcal{L}_{t,s} a) = \{p(t), \mathcal{L}_{t,s} a\}, \quad \mathcal{L}_{s,s} a = a.$$

At the quantum level, one works with the quantization of  $p(t)$ , the operator  $P^h(t)$  and, given an observable  $a$ , one considers the conjugation of the operator  $\text{Op}_h(a)$  by the propagators  $U^h(t, s)$ :

$$U^h(s, t) \circ \text{Op}_h(a) \circ U^h(t, s).$$

The Egorov Theorem connects the classical picture and the quantum one in the limit  $h \rightarrow 0$  (see for instance [81])

**THEOREM.** *There exists a constant  $C > 0$  such that for all  $a \in \mathcal{S}(\mathbb{R}^{2d})$  and  $t, s \in \mathbb{R}$*

$$\begin{aligned} & \left\| U^h(s, t) \circ \text{Op}_h(a) \circ U^h(t, s) - \text{Op}_h(\mathcal{L}_{t,s} a) \right\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \\ & \leq C h^2 |t - s| e^{C|t-s|} N(a), \end{aligned} \quad (23)$$

where  $N(a)$  denotes a fixed semi-norm of  $a$ .

For some  $\delta \in (0, 1)$ , on a large time interval of size  $|t - s| \sim \frac{\delta}{C} \ln(\frac{1}{h})$ , the error estimate in (23) is  $\delta h^{2-\delta} \ln(\frac{1}{h}) N(a) \ll 1$ . This large time for which  $\text{Op}_h(\mathcal{L}_{t,s} a)$  provides a good approximation is called the *Ehrenfest time* and characterizes the range of validity of the semi-classical approximation [11].

#### 3.4.2 Semi-classical measures and propagators

Assume in this section that the Hamiltonian  $p$  does not depend on the time,  $p = p(x, \xi)$ . To study

$$\psi^h(t) := U^h(t, 0) \psi_0^h, \quad h > 0,$$

on (possibly large) time scales  $t \sim 1/h^\alpha$ ,  $\alpha \geq 0$ , one considers the limit as  $h$  goes to 0 of the quantities

$$\int_{\mathbb{R}} \theta(t) \langle W[\psi^h(t/h^\alpha)], a \rangle dt$$

for  $\theta \in L^1(\mathbb{R})$  and  $a \in \mathcal{S}(\mathbb{R}^{2d})$ . Up to the extraction of a subsequence, this limit is described by a family of measures  $d\mu_\alpha^t(x, \xi) \otimes dt$  that is also called a semi-classical measure of the family  $(\psi^h(t/h^\alpha))_{h>0}$ .

The Egorov Theorem implies the following:

**Case  $\alpha = 0$ .** Any semi-classical measure  $d\mu_0^t(x, \xi) \otimes dt$  of  $(\psi^h(t))_{h>0}$  satisfies  $\mu^t = \Phi_*^{t,0} \mu$  for  $\mu$  a semi-classical measure of  $(\psi_0^h)$ .

**Case  $\alpha > 0$ .** Any semi-classical measure  $d\mu_\alpha^t(x, \xi) \otimes dt$  of  $(\psi^h(\frac{t}{h^\alpha}))_{h>0}$  satisfies the invariance property:  $\mu_\alpha^t = \Phi_*^{s,0} \mu_\alpha^t$  for all  $s \in \mathbb{R}$ . In other words, the measure  $\mu_\alpha^t$  is invariant by the flow  $s \mapsto \Phi^{s,0}$ .

When  $\alpha = 0$ , the description of measure given above in this case opens algorithmic strategies for a numerical computation of the Wigner transform of



$(\psi^h(t))_{h>0}$ . At leading order, this Wigner transform is approximated by the Wigner measure, and thus by the pull-back by the flow  $\Phi^{t,0}$  of the Wigner transform of  $(\psi_0^h)_{h>0}$ , that can be computed numerically via a quadrature procedure for the integral (17). The correspondence principle allows to trade the resolution of a  $h$ -dependent PDE by solving  $h$ -independent ODEs [59].

In the case  $\alpha > 0$ , the invariance property of  $\mu_\alpha^t$  implies that  $\text{supp}(\mu_\alpha^t)$  is a union of periodic orbits of the flow. For example, if  $p = |\xi|^2/2$ , the flow  $\Phi^{s,0}$  is given by  $(x, \xi) \mapsto (x + s\xi, \xi)$ ; the fact that the measure  $\mu_\alpha^t$  is of finite mass and invariant by  $\Phi^{s,0}$  implies  $\text{supp}(\mu_\alpha^t) \subset \{\xi = 0\}$ ; this illustrates the dispersion effects in the Schrödinger equation. Such an analysis is at the roots of the results of [7] on the torus, for example.

### 3.4.3 Propagation of coherent states

The propagation of coherent states also illustrates the correspondence principle. For  $z = (q, p) \in \mathbb{R}^{2d}$ , the function  $U^h(t, s)g_z^h$  can be described at leading order via classical quantities. We need to introduce additional notations

One enlarges the set of profiles and considers complex-valued Gaussian profiles  $g^\Gamma$ , whose covariance matrix  $\Gamma$  is taken in the Siegel half-space  $\mathfrak{S}^+(d)$  of  $d \times d$  complex-valued symmetric matrices with positive imaginary part,

$$\mathfrak{S}^+(d) = \left\{ \Gamma \in \mathbb{C}^{d \times d}, \Gamma = {}^t\Gamma, \text{Im } \Gamma > 0 \right\}.$$

More precisely,  $g^\Gamma$  is given by

$$g^\Gamma(x) := c_\Gamma e^{\frac{i}{2}\Gamma x \cdot x}, \quad x \in \mathbb{R}^d, \Gamma \in \mathfrak{S}^+(d),$$

where  $c_\Gamma = \pi^{-d/4} \det^{1/4}(\text{Im } \Gamma)$  is a  $L^2$ -normalization constant.

For  $z = (q, p) \in \mathbb{R}^{2d}$ , set

$$g_z^{\Gamma, h}(x) = h^{-\frac{d}{4}} e^{\frac{i}{h}p \cdot (x-q)} g^\Gamma \left( \frac{x-q}{\sqrt{h}} \right), \quad x \in \mathbb{R}^d.$$

Note that  $g_z^{i\text{Id}_d, h} = g_z^h$ .

We also introduce classical quantities associated with the flow map  $\Phi^{t,s}$  introduced in (22). Firstly, consider the  $d \times d$  blocks of the *Jacobian matrix*  $F(t, s, z) = \partial_z \Phi^{t,s}(z)$

$$F(t, s, z) = \begin{pmatrix} A(t, s, z) & B(t, s, z) \\ C(t, s, z) & D(t, s, z) \end{pmatrix},$$

which satisfies the linearized flow equation

$$\partial_t F(t, s, z) = J \text{Hess}_z p(t, \Phi^{t,s}(z)) F(t, s, z),$$

with  $F(s, s, z) = \text{Id}_{2d}$ . The matrix-valued function  $F$  is smooth in  $t, s, z$  with any derivative in  $z$  bounded.

Secondly, we introduce the *action integral*

$$S(t, s, z) = \int_s^t (\xi(t') \cdot \dot{x}(t') - p(t', z(t'))) dt',$$

where we have set  $z(t) = (x(t), \xi(t)) = \Phi^{t,s}(z)$ .

With this notation, for  $\Gamma \in \mathfrak{S}^+(d)$ , one has in  $L^2(\mathbb{R}^d)$

$$U^h(t, s)g_z^{\Gamma, h} = e^{\frac{i}{h}S(t,s,z)} g_{\Phi^{t,s}(z)}^{\Gamma(t,s,z), h} + O(\sqrt{h}), \quad (24)$$

with

$$\begin{aligned} \Gamma(t, s, z) &= (C(t, s, z) + D(t, s, z)\Gamma) \\ &\quad \times (A(t, s, z) + B(t, s, z)\Gamma)^{-1}. \end{aligned}$$

Having  $\Gamma(t, s, z) \in \mathfrak{S}^+(d)$  follows from (non elementary) algebraic relations. The description can be made more precise with an asymptotic expansion in powers of  $\sqrt{h}$  [23].

The propagation of semi-classical wave packets was also investigated in nonlinear contexts by various authors. Wave packets are flexible enough for some nonlinear superposition results to hold. We refer to the book of R. Carles [16] and the references therein.

### 3.4.4 Semi-classical approximation of the propagator

The description of the propagation of Gaussian states and the formula (7) yield approximation formulae for the propagator that can be used for a numerical determination of  $U^h(t, 0)\psi$ ,  $\psi \in L^2(\mathbb{R}^d)$ .

One defines the action of the *thawed Gaussian approximation* on  $\psi \in L^2(\mathbb{R}^d)$  by

$$\mathcal{I}_{\text{th}}^h(t)\psi = (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} \langle \psi, g_z^h \rangle e^{\frac{i}{h}S(t,0,z)} g_{\Phi^{t,0}(z)}^{h, \Gamma(t,0,z)} dz,$$

and the *frozen Gaussian approximation* by

$$\begin{aligned} \mathcal{I}_{\text{fr}}^h(t)\psi &= (2\pi h)^{-d} \int_{\mathbb{R}^{2d}} \langle \psi, g_z^h \rangle k(t, 0, z) e^{\frac{i}{h}S(t,0,z)} g_{\Phi^{t,0}(z)}^h dz, \end{aligned}$$

with

$$\begin{aligned} k(t, 0, z) &= 2^{-d/2} \det^{1/2} \left( A(t, 0, z) + D(t, 0, z) \right. \\ &\quad \left. + i(C(t, 0, z) - B(t, 0, z)) \right), \end{aligned}$$

which has the branch of the square root determined by continuity in time. The operator  $\mathcal{I}_{\text{fr}}^h(t)$  is often referred to as the *Herman-Kluk propagator*, see [84, 80, 57].

The operators  $\mathcal{I}_{\text{th/fr}}^h(t)$ , built on classical quantities, approximate the unitary propagator  $U^h(t, 0)$ , giving another illustration of the correspondence principle.

**THEOREM** ([84, 80]). *Let  $p(t)$  be a smooth subquadratic Hamiltonian, then for  $h \in (0, 1]$ ,*

$$U^h(t, 0) = \mathcal{I}_{\text{th/fr}}^h(t) + O(h) \quad \text{in } \mathcal{L}(L^2(\mathbb{R}^d)).$$

This result illustrates one of the paradigms of the semi-classical approach, consisting in trading the resolution of oscillating PDEs for that of ODEs.

Note that the thawed/frozen Gaussian operators are order  $h$  approximation of the propagator while the wave packet approximation of (24) is of order  $\sqrt{h}$ . This comes from the structure of the remainder term in (24) and integration in  $z$ . A numerical implementation of this approximation was carried out in [61].

The operators  $\mathcal{I}_{\text{th/fr}}^h(t)$  belong to the class of *Fourier integral operators* (FIO). Designing operators that approximate the dynamics of a semi-classical propagator goes back to the early days of semi-classical analysis, see J. Chazarain [19], B. Helffer and D. Robert [47] and [81], see also the books [93, Chapter 12] or [25].

## 4 Applications

### 4.1 Semi-classical analysis of molecular dynamics

#### 4.1.1 Square integrable families valued in Hilbert spaces

The semi-classical pseudodifferential calculus naturally extends to the space  $L^2(\mathbb{R}^d, \mathcal{H})$  for some Hilbert space  $\mathcal{H}$ , such as  $\mathbb{C}^N$  or  $L^2(\mathbb{T}^d)$  where  $\mathbb{T}^d$  is the  $d$ -dimensional torus, for example. One then proceeds as follows:

- (i) The symbols  $a$  are smooth compactly supported functions from  $\mathbb{R}^d$  into the set  $\mathcal{K}(\mathcal{H})$  of compact operators on  $\mathcal{H}$ ,
- (ii) The semi-classical measures are characterized by a positive measure  $\mu$  and a measurable family  $M$  defined on  $\mathbb{R}^{2d}$  and valued in the set of operators on  $\mathcal{H}$  that are  $d\mu$ -a.e. nonnegative trace-class operators [38].

Then, if  $(\psi^h)_{h>0}$  is uniformly bounded in  $L^2(\mathbb{R}^d, \mathcal{H})$ , the pair  $(M, \mu)$  is a semi-classical measure of  $(\psi^h)_{h>0}$  if, up to a subsequence, for all  $a \in \mathcal{C}_c^\infty(\mathbb{R}^d, \mathcal{K}(\mathcal{H}))$ ,

$$(\text{Op}_h(a)\psi^h, \psi^h) \xrightarrow{h \rightarrow 0} \langle \text{Tr}_{\mathcal{L}(\mathcal{H})}(aM), \mu \rangle.$$

Taking  $\mathcal{H} = L^2(\mathbb{T}^d)$  turns out to be pertinent for the study of periodic problems (see [18]). Taking  $\mathcal{H} = \mathbb{C}^N$  leads to the framework of the Schrödinger equation (2) in the Born-Oppenheimer approximation. The symbols then are matrix-valued and the semi-classical measures are characterized by Hermitian matrices [40].

#### 4.1.2 Molecular dynamics

Consider  $U^h(t)$  the unitary propagator associated with equation (2). Denote by  $\text{sp}V(x)$  the set of the eigenvalues of the self-adjoint matrix  $V(x)$  and let  $\lambda(x)$  be an eigenvalue of  $V(x)$  such that

$$\begin{aligned} \exists \delta_0 > 0, \forall x \in \mathbb{R}^d, \\ \text{dist}(\lambda(x), \text{sp}V(x) \setminus \{\lambda(x)\}) > \delta_0. \end{aligned} \quad (25)$$

Denote by  $\Pi(x)$  the associated (smooth) eigenprojector:

$$V(x)\Pi(x) = \Pi(x)V(x) = \lambda(x)\Pi(x), \quad \forall x \in \mathbb{R}^d.$$

Denote by  $\Phi^t$  the classical flow associated with the scalar Hamiltonian

$$p(x, \xi) = \frac{|\xi|^2}{2} + \lambda(x),$$

as in (21), and denote by  $\mathcal{L}^t$  the associated Liouvillian,  $\mathcal{L}^t : a \mapsto a \circ \Phi^t$ . Matrix-valued aspects are treated by introducing the *parallel transport* of matrices along the flow. Let

$$F(x, \xi) := [\xi \cdot \nabla \Pi(x), \Pi(x)],$$

and consider the unitary transforms  $\mathcal{R}(t, z)$  defined for  $t \in \mathbb{R}$ ,  $z \in \mathbb{R}^{2d}$  by

$$\partial_t \mathcal{R}(t, z) = F(\Phi^t(z)) \mathcal{R}(t, z), \quad \mathcal{R}(0, z) = \text{Id}.$$

The map  $\mathcal{R}(t, z)$  preserves the eigenspaces along the flow and maps a vector  $\vec{V}_0$  which is in the range of  $\Pi_j(x_0)$  to a vector  $\mathcal{R}(t, z_0)\vec{V}_0$  in the range of  $\Pi_j(\Phi_j^t(z_0))$ ,  $z_0 = (x_0, \xi_0)$ .

With these notations in hand, the Egorov Theorem admits the following extension [23] to adiabatic situations.

**THEOREM.** *Assume (25), then there exists a constant  $C > 0$  such that for all  $a \in \mathcal{S}(\mathbb{R}^{2d}, \mathbb{C}^{N,N})$  and  $\theta \in L^1(\mathbb{R})$*

$$\begin{aligned} \left\| \int_{\mathbb{R}} \theta(t) \left( U^h(-t) \circ \text{Op}_h(\Pi a \Pi) \circ U^h(t) \right. \right. \\ \left. \left. - \text{Op}_h(\Pi \mathcal{L}^t(\mathcal{R}(-t) a \mathcal{R}(-t)^*) \Pi) \right) dt \right\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \\ \leq C h N(a), \end{aligned} \quad (26)$$

where  $N(a)$  denotes a fixed semi-norm of  $a$ .

Property (25) is called *adiabaticity*, from the greek *adiabatos* = impassable, because, at leading order, the propagation holds inside the eigenmode defining the Hamiltonian  $p(x, \xi)$ . Note also that the generalization of the Egorov theorem requires averaging in time.

This result extends to general time dependent subquadratic Hamiltonians  $p = p(t, x, \xi)$  with eigenvalues and eigenprojectors that depend simultaneously on the position and momentum variables up to the introduction of classical quantities associated to each eigenvalues [23].

The proof of (26) relies on a diagonalization process using what is called *super-adiabatic projectors*, as carried out by A. Martinez and V. Sordani [71] as well as H. Spohn and S. Teufel [83], see G. Nenciu's work [76] for earlier results. See also [87].

As for scalar equations, one can extend the thawed/frozen Gaussian approximations and construct FIO approximating the propagator  $U^h(t)$  associated with  $P^h$  by using the eigenprojector and the classical quantities associated with the eigenvalues [33]. Let us also mention nonlinear results for systems in [16, 43] and for initial data that are semi-classical wave packets (see also references therein).

### 4.1.3 Eigenvalue crossings

If the adiabatic condition (25) is not satisfied, or if the gap between the eigenvalues shrinks as  $h \rightarrow 0$  (see [42]), transitions between modes may occur. These non adiabatic effects were observed in the early 1930s by L. Landau [58] and C. Zener [92] independently. They were investigated more in details in the 1990's, starting with the work of G. Hagedorn [41] for the equation (2) with Gaussian wave packets for initial data.

For a general Hamiltonian  $H(t, x, \xi)$ , crossings were classified in the early 2000's by Y. Colin de Verdière [21] through a reduction to normal forms. The analysis of the semi-classical measures and Wigner transforms is understood in these generic situations [31, 29, 32]. The loss of adiabaticity led to replace the Liouville operator of Theorem 4.1.2, by a Markov process including branches of classical trajectories and a branching procedure whenever the gap defined in (25) is minimal on a trajectory.

Assume  $d = 2$  and consider the potential

$$V(x) = \begin{pmatrix} w_1(x) & w_2(x) \\ w_2(x) & -w_1(x) \end{pmatrix}.$$

Denoting by  $\Pi_{\pm}$  the eigenprojectors of  $V$ , one has

$$V = \lambda_+ \Pi_+ + \lambda_- \Pi_-, \quad \lambda_{\pm}(x) = \pm \sqrt{w_1(x)^2 + w_2(x)^2}.$$

Eigenvalue crossings occur on the set

$$\Upsilon = \{(x, \xi) \in \mathbb{R}^4, w_1(x) = w_2(x) = 0\}$$

that is a submanifold of  $\mathbb{R}^4$  under the assumption

$$\text{Rk } dw|_{\Upsilon} = 2.$$

The classical trajectories  $\Phi_{\pm}^t$  associated with the Hamiltonian  $\frac{|\xi|^2}{2} + \lambda_{\pm}(x)$  can be continuously continued through points  $(x, \xi) \in \Upsilon$  such that

$$dw(x)\xi := \xi_1 \nabla w_1(x) + \xi_2 \nabla w_2(x) \neq 0_{\mathbb{R}^2}.$$

The gap between the eigenvalues

$$g(x) = 2|w(x)|$$

is minimal along a trajectory when it passes through the hypersurface

$$\Sigma = \{(x, \xi) \in \mathbb{R}^2, w(x) \cdot (dw(x)\xi) = 0\}.$$

This set is called *hoping hypersurface* in the chemical literature because switches between modes occurs on  $\Sigma$ , as we shall see now.

In order to describe the transitions, one considers an extended phase space

$$T_{\pm}^* \mathbb{R}^2 = \mathbb{R}^4 \times \{+1, -1\},$$

and trajectories defined on  $T_{\pm}^* \mathbb{R}^2$  as branches of smooth trajectories  $(\Phi_{\pm}^t)_{t_i \leq t \leq t^*}$  that splits into two trajectories

$$(\Phi_{\pm}^t)_{t^* \leq t \leq t_f} \quad \text{and} \quad (\Phi_{\mp}^t)_{t^* \leq t \leq t_f},$$

whenever  $\Phi_{\pm}^{t^*} \in \Sigma$ . The initial and final times  $t_i$  and  $t_f$  are such that on the time interval  $[t_i, t_f]$  the trajectory only reaches  $\Sigma$  at a single time  $t^*$ . The probability of switching from the mode  $\pm$  to the mode  $\mp$  is given by the *Landau-Zener transition rate*

$$T(x, \xi) = \exp\left(-\frac{\pi}{h} \frac{|w(x)|^2}{|dw(x)\xi|}\right).$$

This generates a random walk characterized by the probability  $\mathbb{P}_{z, \ell, t}(\Gamma)$  of reaching  $\Gamma \subset T_{\pm}^* \mathbb{R}^2$  at time  $t$  starting from the point  $(z, \ell) \in T_{\pm}^* \mathbb{R}^2$ . With this probability law is associated a Markov process  $\mathcal{L}_{\text{LZ}}^t$  on the set of functions defined on  $T_{\pm}^* \mathbb{R}^2$

$$\mathcal{L}_{\text{LZ}}^t f(z, \ell) = \int_{T_{\pm}^* \mathbb{R}^2} f(z', \ell') d\mathbb{P}_{z, \ell, t}(z', \ell').$$

By identifying the set of observables

$$\mathcal{A} = \{a \in \mathbb{C}^{2,2}, a = a_+ \Pi_+ + a_- \Pi_-\}$$

to functions on  $T_{\pm}^* \mathbb{R}^2$  according to

$$(x, \xi, \pm 1) \mapsto a_{\pm}(x, \xi),$$

one extends the actions of  $\mathcal{L}_{\text{LZ}}^t$  to functions of  $\mathcal{A}$ . Then, it is proved in [32] that under reasonable assumptions, if  $\theta \in \mathcal{C}_c^{\infty}(\mathbb{R})$  and  $a \in \mathcal{A}$ ,

$$\left\| \int \theta(t) \left( U^h(-t) \text{op}_h(a) U^h(t) - \text{op}_h(\mathcal{L}_{\text{LZ}}^t a) \right) dt \right\|_{\mathcal{L}(L^2(\mathbb{R}^2))} \leq C h^{1/8}.$$

The proof of this result relies on reduction to normal forms as in [21] and precise analysis of the normal forms. Finding an optimal version of the latter estimate is open.

## 4.2 Geometric aspects and application to quantum limits

We discuss here our second application on the behavior of sequences of eigenfunctions of the Laplace-Beltrami operator of a smooth compact manifold without boundary.

### 4.2.1 Semi-classical analysis on Riemannian manifolds

To extend the semi-classical approach to manifolds, one needs an invariance through change of variables.

With  $\kappa$  a diffeomorphism, from an open set  $U$  into  $V = \kappa(U)$ , is associated the local symplectomorphism

$$\sigma_\kappa : z = (x, \xi) \mapsto (\kappa(x), {}^t d\kappa(x)^{-1}\xi).$$

The map  $\sigma_\kappa$  is associated with the unitary transformation  $J_\kappa$  of  $L^2(\mathbb{R}^d)$

$$J_\kappa f = \text{Jac}(\kappa)^{-\frac{1}{2}} f \circ \kappa^{-1} \in \mathcal{C}_c^\infty(V), \quad f \in \mathcal{C}_c^\infty(U).$$

There exists a constant  $C > 0$  and a semi-norm  $N$  such that for all  $a \in \mathcal{C}_c^\infty(V \times \mathbb{R}^d)$  one has

$$\|J_\kappa^* \text{Op}_h(a) J_\kappa - \text{Op}_h(b)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C h N(a), \quad (27)$$

where  $b = a \circ \sigma_\kappa \in \mathcal{C}_c^\infty(U \times \mathbb{R}^d)$ .

This result allows one to define  $h$ - $\psi$ do on a Riemannian manifolds  $M$  through local charts. However, they are only defined at leading order (up to  $O(h)$  in  $\mathcal{L}(L^2(M))$ ) [93].

Relation (27) also enlightens the geometric structure of semi-classical measures that appear as measures on the cotangent space  $T^*M$ , the bundle above  $M$  whose fibers above  $x \in M$  consists in the dual set of the tangent set  $T_x M$ .

The semi-classical approach can also be extended in the context of (noncommutative) nilpotent graded Lie groups and nilmanifolds (that are quotient of such a group by one of its co-compact subgroup), using the definition of the Fourier transform via representation theory [30], or in infinite dimensional frameworks [1, 2].

### 4.2.2 Quantum limits

With these tools in hand, one can consider a sequence of eigenfunctions  $(\varphi_k)_{k \in \mathbb{N}}$  of the Laplace-Beltrami operator  $-\Delta_M$  on  $M$  as defined in (3). The asymptotics as  $E \rightarrow +\infty$  of the counting function

$$N(E) = \#\{k \in \mathbb{N}, E_k \leq E\}.$$

are described by the *Weyl law* [89, 93]

$$N(E) \sim (2\pi)^{-d} E^{\frac{d}{2}} \text{Vol}(M) \omega_d.$$

Here  $d$  denotes the dimension of  $M$  and  $\omega_d$  is the volume of the Euclidean unit ball in  $\mathbb{R}^d$ . It can be derived from (16), writing

$$N(E) = \|\text{Op}_h(a)\|_{\text{HS}(L^2(M))}^2$$

for  $\text{Op}_h(a) = \chi(-h^2 \Delta_M)$  with  $h = E^{-\frac{1}{2}}$  and  $\chi \in \mathcal{C}_c^\infty(T^*M)$  approaching  $1_{[0,1]}(\xi) 1_M(x)$  [3, 93].

A large literature is devoted to the analysis of the limit as  $E \rightarrow +\infty$  of

$$\frac{1}{N(E)} \sum_{E_k \leq E} \left| \int_M \phi(x) |\varphi_k(x)|^2 dx \right|^2, \quad \phi \in \mathcal{C}^0(M),$$

extended to functions  $a \in \mathcal{C}_c^\infty(T^*M)$  as

$$\nu_E(a) := \frac{1}{N(E)} \sum_{E_k \leq E} \left| \left( \text{Op}_{E^{-\frac{1}{2}}}(a) \varphi_k, \varphi_k \right) \right|^2.$$

The geodesic flow is the Hamiltonian flow associated with the symbol of the Laplace-Beltrami operator  $-\Delta_M$ . Since one deduces (19) and (20) from equation (3), properties of the geodesic flow have consequences for the limits of  $\nu_E(a)$  as  $E \rightarrow +\infty$ .

A flow  $\Phi^t$  is said to be *ergodic* if for Lebesgue almost all  $(x_0, \xi_0) \in T^*M$  and for all  $a \in \mathcal{C}^0(T^*M)$ ,

$$\begin{aligned} & \frac{1}{T} \int_0^T \Phi_*^t a(x_0, \xi_0) dt \\ & \xrightarrow{T \rightarrow +\infty} \int_{S^*M} a(x, |\xi_0| \omega) d\text{Vol}(x) d\sigma_x(\omega). \end{aligned}$$

Here,  $d\text{Vol}(x) = \text{Vol}(M)^{-1} dx$  is the normalized measure on  $M$  and  $d\sigma_x(\omega)$  the measure on the sphere  $S_x^*M$  where  $(x, \omega) \in S^*M$  iff

$$\omega \in S_x^*M := \{\xi \in T^*M, \|\xi\|_x = 1\}.$$

In the formula above,  $\|\cdot\|_x$  denotes the vector norm in  $T_x^*M$ . The result is the following (see [86, 20, 91]).

**THEOREM.** *If the geodesic flow of  $M$  is ergodic, then*

$$\begin{aligned} & \lim_{E \rightarrow +\infty} \frac{1}{N(E)} \sum_{E_k \leq E} \left| \left( \text{Op}_{E^{-\frac{1}{2}}}(a) \varphi_k, \varphi_k \right) - \int_{S^*M} a \left( x, \left( \frac{E_k}{E} \right)^{1/2} \omega \right) d\text{Vol}(x) d\sigma_x(\omega) \right|^2 = 0. \end{aligned}$$

The result has an alternative equivalent version that reduces to considering the average of

$$\begin{aligned} \mathbb{L}(a, E_k) := & \left| \left( \text{Op}_{E_k^{-\frac{1}{2}}}(a) \varphi_k, \varphi_k \right) - \int_{S^*M} a(x, \omega) d\text{Vol}(x) d\sigma_x(\omega) \right|^2 \end{aligned}$$

for eigenvalues  $E_k$  such that  $\frac{E}{2} \leq E_k \leq \frac{3E}{2}$ . One then has

$$\lim_{E \rightarrow +\infty} \frac{1}{N(\frac{3E}{2}) - N(\frac{E}{2})} \sum_{\frac{E}{2} \leq E_k \leq \frac{3E}{2}} \mathbb{L}(a, E_k) = 0. \quad (28)$$

At that level, the semi-classical aspects are easier to see. Indeed, (3) shows that the family  $(\varphi_k)_{k \in \mathbb{N}}$  is  $E_k^{-\frac{1}{2}}$ -oscillating, which motivates to adopt a semi-classical setting with  $h_k = E_k^{-\frac{1}{2}}$ . The localization property (19) implies that the support of any semi-classical measure of  $(\varphi_k)_{k \in \mathbb{N}}$  is supported in  $S^*M$  and the limit in (28) is the semi-classical one since  $E_k \sim E$  therein. Besides, the propagation result (20) implies the invariance of the semi-classical measures of sequences  $(\varphi_k)_{k \in \mathbb{N}}$  under the geodesic flow. When this flow is ergodic the only measure invariant under the geodesic flow is the Liouville measure, which restricts the set of quantum limits to the Liouville measure.

The result is even stronger. Indeed, one of its consequence consists in the existence of a set  $S \subset \mathbb{N}$  of density 1, meaning a set satisfying

$$\frac{\#\{k \in S, E_k \leq E\}}{N(E)} \xrightarrow{E \rightarrow +\infty} 1$$

such that

$$\left( \text{Op}_{E_k^{-\frac{1}{2}}}(a) \varphi_k, \varphi_k \right) \xrightarrow{k \rightarrow +\infty, k \in S} \int_{S^*M} a(x, \omega) d\text{Vol}(x) d\sigma_x(\omega). \quad (29)$$

The *unique quantum ergodicity conjecture* of Z. Rudnick and P. Sarnak [82] predicts that the limit in (29) holds for the full sequence, see N. Anantharaman's book [3].

More generally, the relation between the geometry of the manifolds and the nature of quantum limits has been the subject of intensive research during the last decades (see [44, 5, 26, 27, 8, 7, 69, 52] among others), while similar problematic arose in other settings (for sub-Laplacian [22] and on random graphs [6] for example).

### 4.3 Semi-classical methods in control theory

With the notations of the preceding paragraph, for  $n \in \mathbb{N}^*$  set  $J_n = \{k; 2^{n-2} < \sqrt{E_k} < 2^{n+2}\}$ , and denote by  $\mathcal{F}_n$  the set of functions of the form

$$u(t, x) = \sum_{k \in J_n} e^{it\sqrt{E_k+1}} u^k \varphi_k(x),$$

for the coefficients  $u^k \in \mathbb{C}$ . They are solutions to the wave equation (4) with a time-frequency  $\tau \sim 2^n$ . Set the semi-classical parameter to be  $h_n = 2^{-n}$ .

Suppose  $T > 0$  and  $\omega$  is an open subset of  $M$ . Suppose there exist  $C > 0$  and  $n_0 \in \mathbb{N}^*$  such that for all  $n \geq n_0$  and all  $u \in \mathcal{F}_n$  one has

$$\mathcal{E}(u) \leq C \int_0^T \|1_\omega \partial_t u\|_{L^2(M)}^2 dt, \quad (30)$$

that is, observability for those frequency-localized solutions; see (5) where observability is defined. Then, the wave equation (4) is observable from  $\omega$  in time  $T > 0$ , and exact controllability follows. One calls estimate (30) a *semi-classical observability inequality*. We discuss conditions for its validity in the next Section 4.3.1.

The proof of this extension of observability to all solutions to the wave equation in [64, 13] makes use of the following unique continuation property

$$-\Delta_M \varphi = \mu \varphi \quad \text{and} \quad \varphi|_\omega = 0 \quad \Rightarrow \quad \varphi = 0. \quad (31)$$

A now classical tool to prove such a result is a Carleman estimate that can be viewed as a sub-elliptic semi-classical estimate; these estimates are presented in Section 4.3.2.

In fact, the semi-classical observability estimate (30) takes care of the high-frequency component of the solutions, while the unique continuation properties handles the remaining low frequencies.

#### 4.3.1 Geometric control condition

To analyse observability issues, it is classical to adopt a space-time point of view and to work in the variables

$$(t, x, \tau, \xi) \in T^*(\mathbb{R}_t \times M_x).$$

One can have intuitions based on geometrical optics and propagation of energy along rays to support this point of view. This intuition turns out to be correct as explained below.

The symbol of the wave operator is

$$p(x, \tau, \xi) = -\tau^2 + g_x(\xi, \xi)$$

in local coordinates. The Hamiltonian curves (rays) of the space-time Hamiltonian  $p$  are called *bicharacteristic curves*. Their projections on  $M$  are the *geodesics*.

The semi-classical observability estimate (30) is proven to hold under the following property: any bicharacteristic reaches a point above  $]0, T[ \times \omega$ . This condition is called the *geometric control condition* (GCC). Equivalently it reads: any geodesic travelled at speed one enters the observation region  $\omega$  in a time less than  $T$ . Then, assuming (GCC), the proof

of (30) can be carried out by contradiction. Suppose  $U = (u_n)_{n \in \mathbb{N}^*}$  is a sequence with  $u_n \in \mathcal{F}_n$  such that

$$h_n^2 \mathcal{E}(u_n) \sim 1 \quad \text{and} \quad \int_0^T \|1_\omega h_n \partial_t u_n\|_{L^2(M)}^2 dt \rightarrow 0, \quad (32)$$

as  $n \rightarrow +\infty$ . Then  $\|u_n(t, \cdot)\|_{L^2(M)} \sim 1$  and associated with a subsequence of  $U$  is a semi-classical measure  $\mu$ . Note that  $U$  is bounded in  $L^2_{\text{loc}}(\mathbb{R}_t; L^2(M))$  here. The measure is thus understood acting on functions compactly supported in the variable  $t$ . On the one hand, one has

$$h_n \|\nabla_x u_n(t, \cdot)\|_{L^2(M)} \sim h_n \|\partial_t u_n(t, \cdot)\|_{L^2(M)} \sim 1,$$

implying that  $U$  is  $h_n$ -oscillating. One deduces that  $\mu$  has positive mass. On the other hand, the second part of (32) gives  $\mu = 0$  above  $]0, T[ \times \omega$ .

With Section 3.3.4, one finds that  $\text{supp}(\mu) \subset \text{Char}(p)$  and  $H_p \mu = 0$  in the sense of distributions, meaning that  $\mu$  is invariant along the bicharacteristic flow. By the GCC, all bicharacteristics enter the region above  $]0, T[ \times \omega$  where  $\mu$  vanishes implying that  $\mu = 0$ . A contradiction.

Arguments are more involved in the case of a manifold with boundary and a wave equation formulated with a boundary condition, say the homogeneous Dirichlet condition. Away from the boundary, the measure equation  $H_p \mu = 0$  holds. At the boundary, one can derive a measure equation that includes a source term associated with the semi-classical measure of the Neumann trace. This source term generates transport of the measure  $\mu$  along the Melrose-Sjöstrand generalized bicharacteristics [74]. Those obey the laws of geometrical optics: reflection if the boundary is hit transversally, possible glancing and gliding if the boundary is hit tangentially. The GCC remains unchanged apart from exchanging bicharacteristics with generalized bicharacteristics and the observability/exact controlability result holds under this condition.

The proof of wave observability with the sharp GCC condition was first given by C. Bardos, G. Lebeau, and J. Rauch [9], in the case of smooth coefficients with microlocal techniques based on the propagation of singularities. The use of measures was initiated by N. Burq and P. Gérard to further explain the necessary and sufficient aspects of the GCC [12]. One interest of the use of semi-classical measures is the possibility of lowering the regularity of the coefficients. In [14, 15], this regularity is pushed down to a  $\mathcal{C}^1$ -metric on a  $\mathcal{C}^2$ -manifold with boundary. Then, the Hamiltonian vector field  $H_p$  is only continuous. Generalized bicharacteristics exist but uniqueness is lost. Yet, the GCC makes sense

and despite the absence of flow one proves that the support of the semi-classical measure  $\mu$  is a union of generalized bicharacteristics, allowing one to conclude the contradiction argument as above.

### 4.3.2 Carleman estimates as sub-elliptic semi-classical estimates and unique continuation

For a second-order elliptic operator  $P$ , a *Carleman estimate* takes the form, for some  $C > 0$ ,

$$h^{1/2} (\|e^{\varphi/h} u\|_{L^2} + \|e^{\varphi/h} h \nabla_x u\|_{L^2}) \leq C \|h^2 e^{\varphi/h} P u\|_{L^2}, \quad (33)$$

for  $u$  smooth with compact support. The inequality holds if the function  $\varphi$ , called the *weight function*, is well chosen and if  $0 < h \leq h_0$ , for  $h_0$  sufficiently small. For  $x_0 \in \mathbb{R}^d$ , a possible choice of weight function is

$$\varphi(x) = \exp(-\gamma|x - x_0|).$$

Given any  $c_0 > 0$ , estimate (33) holds for functions  $u$  supported in the annulus  $0 < c_0 \leq |x - x_0| \leq 4c_0$  if  $\gamma > 0$  is chosen large [53, 62, 63]. For  $a > 0$ , set  $B_a = \{x \in \mathbb{R}^d, |x - x_0| \leq a\}$  and  $B' = B_{4c_0}$ . Then, for  $c_0 < r < 2c_0$  one deduces from (33) the existence of  $C > 0$  and  $\delta \in ]0, 1[$  such that

$$\|u\|_{H^1(B_{2r})} \leq C \|u\|_{H^1(B')}^{1-\delta} (\|P u\|_{L^2(B')} + \|u\|_{H^1(B_r)})^\delta.$$

This is a quantification of the unique continuation property: if  $u = 0$  in  $B_r$  and  $P u = 0$  then  $u = 0$  in  $B_{2r}$ . Applied to  $P = -\Delta_M - \mu$ , one obtains (31).

Estimate (33) is equivalent to

$$h^{1/2} (\|v\|_{L^2} + \|h \nabla_x v\|_{L^2}) \lesssim \|P_\varphi v\|_{L^2}, \quad (34)$$

where  $P_\varphi = h^2 e^{\varphi/h} P e^{-\varphi/h}$  is a semi-classical differential operator. This operator fails to be elliptic in general, yet the weight function  $\varphi$  is chosen so that the following property holds for  $p_\varphi$ , the symbol of  $P_\varphi$ ,

$$p_\varphi(x, \xi) = 0 \quad \Rightarrow \quad \{\text{Re } p_\varphi, \text{Im } p_\varphi\} = \frac{1}{2i} \{\overline{p_\varphi}, p_\varphi\} > 0,$$

that is, a subellipticity property. This explains the factor  $h^{1/2}$  on the left-hand side of (33) that expresses a half-derivative loss as compared to an elliptic estimate. One proves

$$\nu |p_\varphi|^2(x, \xi) + \{\text{Re } p_\varphi, \text{Im } p_\varphi\}(x, \xi) \geq C(1 + |\xi|^4),$$

and (34) follows from the sharp Gårding inequality (13).

Carleman inequalities can be derived for other types of operators and under fine geometrical properties between the operator  $P$  and the weight function  $\varphi$ , so-called pseudo-convexity conditions. The reader is referred to [66] for an exposition.

## 5 Concluding remark

In the 1970s, people from the microlocal community started to show a strong interest in semi-classical analysis. Let us mention some of the first contributions on the domain by V. Maslov [72] and A. Voros [88]. Fifty years later, the theory has grown considerably. Taking the correspondence principle as a guideline, the authors aimed to show how vast the field of applications of semi-classical is today. The authors hope they have managed to pass on their interest and enthusiasm for semi-classical analysis through striking results. The different examples presented here reflect the mathematical tastes of the authors and should not be thought as exhaustive. They recommend the reading of the section devoted to semi-classical analysis by B. Helffer in the previous edition of this encyclopedia, his commented bibliography [45]; the books by M. Zworski [93] and by M. Dimassi and J. Sjöstrand [25] will be useful for both junior and confirmed researchers.

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