SEMI-CLASSICAL ANALYSIS AND WAVE PACKETS

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Abstract. This text consists in the lectures notes of a course given in Nantes in January - March 2026. We explain the semi-classical approach and focus on wave packets (coherent states), in the aim of constructing a Fourier integral operator that approximates the propagator of a semiclassical Schrödinger equation.

Contents

1. Introduction

This lecture aims at connecting two fields that have known major developments during the last century: the microlocal approach of semiclassical analysis and the analysis on Nilpotent Lie groups.

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 particule by the simultaneous knowledge of its position and its impulsion. This is expressed by the Heisenberg uncertainty principle that we first discuss.

1.1. **Uncertainty principle.** In quantum mechanics, a particule is described by a probability measure $|\psi(x)|^2dx$, with ψ a normalized square integrable function on the configuration space $\mathbb{R}^d_x$, called its *wave function*. Denoting by x_j the coordinates of $x \in \mathbb{R}^d$, the *average position* of the particule is the expectation value of the observables x_j

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

Similarly, the *average impulsion* is

$$\langle \xi_j\rangle_\psi = \int_{\mathbb{R}^d} \hbar D_{x_j}\psi(x)\,\overline{\psi}(x)dx = \int_{\mathbb{R}^d} \hbar\xi_j|\widehat{\psi}(\xi)|^2\frac{d\xi}{(2\pi)^d},\quad D_{x_j} = \frac{1}{i}\partial_{x_j},$$

where we have used the Plancherel theorem for the Fourier transform. Considering the variance of these expectation values,

$$\begin{aligned}(d_\psi x_j)^2 &= \langle (x_j - \langle x_j\rangle_\psi)^2\rangle_\psi = \int_{\mathbb{R}^d}(x_j - \langle x_j\rangle_\psi)^2|\psi(x)|^2dx,\\ (d_\psi \xi_j)^2 &= \langle (\xi_j - \langle \xi_j\rangle_\psi)^2\rangle_\psi = \int_{\mathbb{R}^d}(\xi_j - \langle \xi_j\rangle_\psi)^2|\widehat{\psi}(\xi)|^2\frac{d\xi}{(2\pi)^d},\end{aligned}$$

the *Heisenberg uncertainty principle* reads

$$d_\psi x_j\, d_\psi \xi_j \ge \frac{\hbar}{2},\ \ 1 \le j \le d. \tag{1.1}$$

This results from the Cauchy-Schwarz inequality

$$\left|\Im\left((x_j - \langle x_j\rangle_\psi)\psi\ ,\ (\hbar D_{x_j} - \langle \xi_j\rangle_\psi)\psi\right)_{L^2}\right| \le \|(x_j - \langle x_j\rangle_\psi,)\psi\|_{L^2}\|(\hbar D_{x_j} - \langle \xi_j\rangle_\psi)\psi\|_{L^2} = d_\psi x_j\, d_\psi\xi_j,$$

and the observation

$$\Im\left((x_j - \langle x_j\rangle_\psi)\psi, (\hbar D_{x_j} - \langle \xi_j\rangle_\psi)\psi\right)_{L^2} = \frac{1}{2i}\left(\left[\hbar D_{x_j} - \langle \xi_j\rangle_\psi\ ,\ x_j - \langle x_j\rangle_\psi\right]\psi, \psi\right)_{L^2} = -\frac{\hbar}{2}.$$

The Planck constant $\hbar$ reflects the difference between quantum and classical mechanics, since, in the latter, the position and the impulsion are deterministic variables that can be known with precision. The subject of semi-classical analysis is to understand how one can derive classical mechanics from quantum mechanics, by letting the obstruction $\hbar$ go to 0, even though $\hbar$ is a physical constant. Semi-classical analysis has led to the development of asymptotic technics that are now used in various fields of applied mathematics. For this reason, we will skip the notation $\hbar$ and denote ε a small parameter that is present in some problems of interest involving PDEs. Carrying a semi-classical analysis of a problem consists in investigating the properties of a phenomenon of interest in the limit $\varepsilon \to 0$, when ε is a small parameter present in the equation.

1.2. **Gaussian wave packets.** The uncertainty principle is optimal in the sense that there exists a unique family among L^2-functions that saturates the uncertainty principle. This family consists in *Gaussian wave packets*. They are wave functions associated with a classical state $z = (q, p) \in \mathbb{R}^{2d}$ according to

$$g^\varepsilon_z(x) = (\pi\varepsilon)^{-d/4}\exp(-\tfrac{1}{2\varepsilon}|x-q|^2 + \tfrac{i}{\varepsilon}p\cdot(x-q)),\qquad x \in \mathbb{R}^d. \tag{1.2}$$

It is normalized, $\|g^\varepsilon_z\|_{L^2} = 1$, and centered in z,

$$\langle x_j\rangle_{g^\varepsilon_z} = q_j\ \text{ and }\ \langle \xi_j\rangle_{g^\varepsilon_z} = p_j,\ \ 1 \le j \le d,$$

and saturates the uncertainty principle:

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

Gaussian wave packets have the property of being very localized in the sense that if $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} \phi(x) |g_z^\varepsilon(x)|^2 dx = \phi(q) + O(\sqrt{\varepsilon}). \tag{1.3}$$

They also have this property in Fourier variable

$$\int_{\mathbb{R}^d} \phi(\varepsilon D_x) g_z^\varepsilon(x) \overline{g}_z^\varepsilon(x) dx = \phi(p) + O(\sqrt{\varepsilon}), \tag{1.4}$$

where $\phi(\varepsilon D)$ is the *Fourier multiplier* defined by $\widehat{\phi(\varepsilon D) f} = \phi(\varepsilon\xi)\widehat{f}(\xi)$. This results from the fact that, after rescaling , the Fourier transform of g_z^ε has the same Gaussian structure

$$\varepsilon^{-\frac{d}{2}}\, \mathrm{e}^{i\frac{p\cdot q}{2\varepsilon}}\, \widehat{g_z^\varepsilon}\left(\frac{\xi}{\varepsilon}\right) = \mathrm{e}^{i\frac{(-p)\cdot q}{2\varepsilon}} g_{Jz}^\varepsilon, \quad Jz = (-p, q) \in \mathbb{R}^{2d}.$$

The relations (1.3) and (1.4) suggest that the phase-space point $z = (q, p)$ is the only obstruction to the strong convergence to 0 in $L^2(\mathbb{R}^d)$ of the sequence g_z^ε: if $\phi(q) = 0$, then ϕg_z^ε converges strongly to 0, and similarly, if $\phi(p) = 0$, then $\phi(\varepsilon D) g_z^\varepsilon$ too.

The family g_z^ε is also said to be *ε-oscillating* because the L^2-norm of its derivatives are of size $O(\frac{1}{\varepsilon})$. It is these oscillations of size $\frac{1}{\varepsilon}$ that prevent strong-convergence. Similar questions can be asked for any bounded family in $L^2(\mathbb{R}^d)$. We will be concerned with such questions.

1.3. **Semiclassical pseudodifferential operators.** The previous analysis of the Gaussian wave packets suggests that the description of oscillating families requires a simultaneous analysis in position and in a rescaled Fourier variables. The theory of semi-classical pseudodifferential operators provided a tool for performing such a program. The quantization problem, or how to associate an operator to an energy, also called Hamiltonian, is a question from quantum mechanics. It gives a mathematical setting for exploring the correspondence between classical and quantum mechanics, and analyzing oscillating phenomena.

Let $a(x, \xi)$ be a *semi-classical observable*, i.e. a function of the Schwartz space $\mathcal{S}(\mathbb{R}^{2d})$. The *semi-classical pseudodifferential operator* of symbol a is the operator $\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)$ defined by

$$\mathrm{op}_\varepsilon^{\mathrm{KN}}(a) f(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a\big(x, \xi\big) \mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)} f(y) dy\, d\xi, \ \ f \in \mathcal{S}(\mathbb{R}^d), \ \ x \in \mathbb{R}^d. \tag{1.5}$$

This form is called the *classical quantization*, also called *Kohn-Niremberg quantization*, of the symbol a [4, 25]. Other types of quantization are possible, like the 'left' quantization, where the symbol appears in the form $a(y, \xi)$, or the Weyl quantization that has the advantage to be symmetric [14, 25]. Such classes of operators enjoy properties that we will study: symbolic calculus for the composition and the adjoint, almost-positiviy, for example.

The action of semiclassical pseidodifferential operators allow to recover the obstruction to strong convergence. For example, when considering Gaussian wave packets, one has

$$(\mathrm{op}_\varepsilon^{\mathrm{KN}}(a) g_z^\varepsilon, g_z^\varepsilon)_{L^2} \underset{\varepsilon\to 0}{\longrightarrow} a(z).$$

The quantity $(\mathrm{op}_\varepsilon^{\mathrm{KN}}(a) g_z^\varepsilon, g_z^\varepsilon)_{L^2}$ also writes

$$(\mathrm{op}_\varepsilon^{\mathrm{KN}}(a) g_z^\varepsilon, g_z^\varepsilon)_{L^2} = \int a(x, \xi) W^\varepsilon[g_z^\varepsilon](x, \xi) dx d\xi.$$

where $W^\varepsilon[g_z^\varepsilon]$ can be proved to be a distribution, i.e. an element of $\mathcal{S}'(\mathbb{R}^{2d})$. Since [24], one calls it the *Wigner transform* of the family $(g_z^\varepsilon)_{\varepsilon>0}$. It converges in the sense of distribution to the Dirac mass in $z = (q, p)$. The latter is said to be a *semi-classical measure*, or a *Wigner measure* of the family $(g_z^\varepsilon)_{\varepsilon>0}$. It characterize the obstruction to the strong convergence of $(g_z^\varepsilon)_{\varepsilon>0}$. We will develop these tools in a general setting.

1.4. **Correspondence principle.** The tools developed above can be combined with evolution problems. Consider a real-valued Hamiltonian H, for example

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

for some nice function V. At the classical level, one associates with h the Newtonian trajectories

$$z \mapsto \Phi^t(z) = (q(t), p(t))$$

such that

$$\dot{q}(t) = \nabla_\xi H(q(t), p(t)), \;\; \dot{p}(t) = -\nabla_x H(q(t), p(t)),$$

with initial value $(q(0), p(0)) = z = (q, p) \in \mathbb{R}^{2d}$. At the quantum level, one considers the operator $\mathrm{op}_\varepsilon(H)$. Then, setting

$$\psi^\varepsilon(t, x) = \mathrm{e}^{\frac{it}{\varepsilon}\,\mathrm{op}_\varepsilon(H)} g_z^\varepsilon(x), \;\; (t, x) \in \mathbb{R} \times \mathbb{R}^d,$$

we have

$$\left(\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)\psi^\varepsilon(t), \psi^\varepsilon(t)\right) \underset{\varepsilon\to 0}{\longrightarrow} a(\Phi^t(z)), \;\; \forall a \in \mathcal{S}(\mathbb{R}^{2d}), \;\; \forall t \in \mathbb{R},$$

showing the classical mechanics derives from the quantum evolution in the semiclassical limit.

2. SEMICLASSICAL ANALYSIS

We present here three concepts that will be central in our approach: semiclassical pseudodifferential operators with smoothing symbol, semiclassical measures and wave packets. We use the Kohn-Niremberg quantization.

2.1. **Semiclassical pseudodifferential operators.** Let $a(x,\xi)$ be a *semi-classical observable*, i.e. a function of the Schwartz space $\mathcal{S}(\mathbb{R}^{2d})$. Using Weyl quantization, the *semi-classical pseudodifferential operator* of symbol a is the operator $\mathrm{op}_\varepsilon(a)$ defined on functions $f\in\mathcal{S}(\mathbb{R}^d)$ by

$$\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)f(x)=(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}a\big(x,\xi\big)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)}f(y)dy\,d\xi. \tag{2.1}$$

The operator $\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)$ maps $\mathcal{S}(\mathbb{R}^d)$ into itself and, by duality, $\mathcal{S}'(\mathbb{R}^d)$ into itself. Its kernel k_ε can be expressed in terms of the inverse Fourier transform of a in the variable ξ

$$\kappa_x(v)=(2\pi)^{-d}\int_{\mathbb{R}^d}a(x,\xi)\mathrm{e}^{i\xi\cdot v}d\xi,\ \ (x,v)\in\mathbb{R}^{2d}, \tag{2.2}$$

or, equivalently, $\widehat{\kappa}_x=a(x,\cdot)$. Indeed, one has

$$k_\varepsilon(x,y)=\frac{1}{\varepsilon^d}\,\kappa_x\left(\frac{x-y}{\varepsilon}\right),\ \ (x,y)\in\mathbb{R}^{2d}.$$

The function κ_x is called the convolution kernel of a, and we the function $(x,v)\mapsto\kappa_x(v)$ is in $\mathcal{S}(\mathbb{R}^{2d})$. As a consequence of the Schur Lemma, we have the following result, which implies that the map $a\mapsto\mathrm{op}_\varepsilon(a)$ is continuous from $\mathcal{S}(\mathbb{R}^{2d})$ into $\mathcal{L}(L^2(\mathbb{R}^d))$.

Proposition 2.1. *The operator* $\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)$ *maps* $L^2(\mathbb{R}^d)$ *into itself and*

$$\|\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\leq\int_{\mathbb{R}^d}\sup_{x\in\mathbb{R}^d}|\kappa_x(v)|dv$$

for $C>0$ *independent of* $a\in\mathcal{S}(\mathbb{R}^{2d})$ *and* $\varepsilon>0$.

Note that this proposition implies that as soon as the convolution kernel κ associated with a symbol a is such that

$$\int_{\mathbb{R}^d}\sup_{x\in\mathbb{R}^d}|\kappa_x(v)|dv<+\infty,$$

one can define the bounded operator $\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)$ on $L^2(\mathbb{R}^d)$. We will use this observation all along this chapter, in particular for evaluating the norm of operators.

2.1.1. *Link between different quantizations.* As mentioned in the introduction different choices of quantization are possible and actually used in practice. They reduce to the choice of a value of $t\in[0,1]$ in the *t-quantization* defined by

$$\forall f\in\mathcal{S}(\mathbb{R}^d),\ \ \mathrm{op}_\varepsilon^t(a)f(x)=(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}a\left(tx+(1-t)y,\xi\right)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)}f(y)dy\,d\xi. \tag{2.3}$$

The choice of $t=1/2$ corresponds to the Weyl quantization, while the choice of $t=1$ gives Kohn–Nirenberg (or classical) quantization and $t=0$, anti Kohn–Nirenberg quantization.

Proposition 2.2. *There exists a constant* $c>0$ *such that for* $t\in[0,1]$, $a\in\mathcal{S}(\mathbb{R}^{2d})$, *we have in* $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\|\mathrm{op}_\varepsilon^{KN}(a)-\mathrm{op}_\varepsilon^t(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\leq c\,\varepsilon\int_{\mathbb{R}^d}\sup_{X\in\mathbb{R}^d}|v\cdot\nabla_x\kappa(X,v)|\,dv,$$

where κ *is given by* (2.2)

Proof. We consider κ the convolution kernel of a and we observe that the kernel of the operator $\mathrm{op}_\varepsilon^t(a)$ is the function

$$(x,y)\mapsto \varepsilon^{-d}\kappa_x^{t,\varepsilon}\big(\tfrac{x-y}{\varepsilon}\big),\ \ \kappa_x^{t,\varepsilon}(v)=\kappa_{x-\varepsilon(1-t)v}(v).$$

Thanks to Taylor formula, one can write

$$\kappa_x^{t,\varepsilon}(v)=\kappa_x(v)-\varepsilon(1-t)B_\varepsilon(x,v),$$
$$\text{with } \ B_\varepsilon(x,v)=v\cdot\int_0^1\nabla_x\kappa_{x-\varepsilon s(1-t)v}(v)ds.$$

Therefore, $\mathrm{op}_\varepsilon^t(a)=\mathrm{op}_\varepsilon^{\rm KN}(a)-\varepsilon(1-t)R_\varepsilon$, where R_ε is the operator of kernel

$$r_\varepsilon(x,y)=\varepsilon^{-d}B_\varepsilon\big(x,\tfrac{1}{\varepsilon}(x-y)\big).$$

One obtains

$$\|R_\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\leq\int_{\mathbb{R}^d}\sup_{x\in\mathbb{R}^d}\big|B_\varepsilon(x,v)\big|dv\leq\int_{\mathbb{R}^d}\sup_{x\in\mathbb{R}^d}\left|v\cdot\nabla_x\kappa_x(v)\right|dv$$

□

Revisiting the proof, we see that we could write an asymptotic expansion at any order in ε for the difference between two quantizations by pushing the Taylor formula at higher order.

2.1.2. *Symbolic calculus.* The set of pseudodifferential operators is an algebra that enjoys symbolic calculus. In view of the preceding section, it is also true for the other quantizations.

Proposition 2.3. *Let $a,b\in\mathcal{S}(\mathbb{R}^{2d})$, then in $\mathcal{L}(L^2(\mathbb{R}^d))$,*

$$\mathrm{op}_\varepsilon^{\rm KN}(a)\mathrm{op}_\varepsilon^{\rm KN}(b)=\mathrm{op}_\varepsilon^{\rm KN}(ab)+\frac{\varepsilon}{i}\,\mathrm{op}_\varepsilon^{\rm KN}\left(\nabla_\xi a\cdot\nabla_x b\right)+O\left(\varepsilon^2\right).$$

Regarding the adjoint, one has in $\mathcal{L}(L^2(\mathbb{R}^d))$

$$\mathrm{op}_\varepsilon^{\rm KN}(a)^*=\mathrm{op}_\varepsilon^{\rm KN}(\overline{a})+\frac{\varepsilon}{i}\,\mathrm{op}_\varepsilon^{\rm KN}\left(\nabla_\xi\cdot\nabla_x a\right)+O\left(\varepsilon^2\right).$$

Here again, the proof will show that one can get asymptotics at any order for these operators.

A convenient manner to prove this proposition consists in using *amplitudes.* We call amplitude any function $\tau\in\mathcal{S}(\mathbb{R}^{3d})$ that we quantize as follows:

$$\mathrm{Aop}_\varepsilon(\tau)f(x)=(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}a\big(x,y,\xi\big)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)}f(y)dy\,d\xi.$$

Then, there exists a constant $C>0$ such that for all $\tau\in\mathcal{S}(\mathbb{R}^{3d})$,

$$\|\mathrm{Aop}_\varepsilon(\tau)\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\leq C\int_{\mathbb{R}^d}\sup_{x,y\in\mathbb{R}^d}|\kappa_\tau(x,y,v)|dv,\qquad \kappa_\tau(x,y,v)=(2\pi)^{-d}\int_{\mathbb{R}^d}\mathrm{e}^{i\xi\cdot v}a(x,y,\xi)d\xi.$$

Here again, the calculus can be extended to amplitudes $\tau(x,y,\xi)=\widehat{\kappa}(x,y,v)$ such that

$$\int_{\mathbb{R}^d}\sup_{x,y\in\mathbb{R}^d}|\kappa_\tau(x,y,v)|dv<+\infty.$$

This may happen for example when $\xi\mapsto\tau(x,y,\xi)$ is Schwartz class uniformly with respect to x and y, without further differentiation properties in x and y..

The link between these quantizations is given by the following lemma.

Lemma 2.4. *Let $\tau\in\mathcal{S}(\mathbb{R}^{3d})$, then in $L^2(\mathbb{R}^d)$,*

$$\mathrm{Aop}_\varepsilon(\tau)=\mathrm{op}_\varepsilon^{\rm KN}(\tau_{|y=x})-i\,\varepsilon\,\mathrm{op}_\varepsilon^{\rm KN}\left(\nabla_y\cdot\nabla_\xi\tau_{|y=x}\right)+O(\varepsilon^2).$$

Proof. We write $\mathrm{Aop}_\varepsilon(\tau) = \mathrm{op}_\varepsilon^{\mathrm{KN}}(a^\varepsilon)$, with $a^\varepsilon(x,\cdot) = \widehat{\kappa}_x^\varepsilon$,

$$\kappa_x^\varepsilon(v) = \kappa(x, x - \varepsilon v, v), \;\; \forall x, v \in \mathbb{R}^d.$$

A Taylor formula gives

$$\kappa_x^\varepsilon(v) = \kappa(x,x,v) - \varepsilon v \cdot \nabla_y \kappa(x,x,v) + \frac{\varepsilon^2}{2} \int_0^1 d_y^2 \kappa(x, x - \varepsilon s v, v) v \cdot v (1-s) ds.$$

We conclude by observing that

$$v \cdot \nabla_y \kappa(x,x,v) = i(\widehat{\nabla_y \cdot \nabla_\xi \tau})(x,x,v).$$

□

We are now in position of proving Proposition 2.3.

Proof of Proposition 2.3. We first observe

$$\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)^* = \mathrm{Aop}_\varepsilon(b), \;\; b(x,y,\xi) = a(y,\xi)$$

and Lemma 2.4 implies the formula for the adjoint in Proposition 2.3. For dealing with the composition, we observe that it is enough to settle an asymptotic formula at order two for $\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)\mathrm{op}_\varepsilon^{\mathrm{KN}}(b)^*$. We have

$$\mathrm{op}_\varepsilon^{\mathrm{KN}}(a)\mathrm{op}_\varepsilon^{\mathrm{KN}}(b)^* = \mathrm{Aop}_\varepsilon(\tau), \;\; \tau(x,y,\xi) = a(x,\xi)\overline{b}(y,\xi),$$

and Lemma 2.4 implies the formula for the composition in Proposition 2.3. □

2.2. **Gårding inequality and semi-classical measures.**

2.2.1. *Bargmann transform.*

We associate with the family $(g_z^\varepsilon)_{\varepsilon>0}$ the Bargmann transform of a function $f \in \mathcal{S}(\mathbb{R}^d)$ ([2]):

$$\mathcal{B}^\varepsilon[f] = (2\pi\varepsilon)^{-\frac{d}{2}} \left(f, g_z^\varepsilon\right)_{L^2}, \;\; z \in \mathbb{R}^{2d}. \tag{2.4}$$

This transform is an isometry from $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$

$$f = (2\pi\varepsilon)^{-\frac{d}{2}} \int_{\mathbb{R}^{2d}} \mathcal{B}^\varepsilon[f](z) g_z^\varepsilon dz, \tag{2.5}$$

Moreover

$$\|f\|^2_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} |\mathcal{B}^\varepsilon[f](z)|^2 dz.$$

2.2.2. *Wick quantization.*

We define the semi-classical Wick quantization for $a \in \mathcal{S}(\mathbb{R}^{2d})$ by conjugating bu the Bargmann transform the operator in $L^2(\mathbb{R}^{2d})$ given by the multiplication by the function $a(z)$

$$\mathrm{op}_\varepsilon^{\mathrm{Wick}}(a) := \mathcal{B}^{\varepsilon,*} a \, \mathcal{B}^\varepsilon.$$

By construction, this quantization is positive.

The integral kernel of $\mathrm{op}_\varepsilon^{\mathrm{Wick}}(a)$ is the function $k_\varepsilon(x,y)$ given by

$$k_\varepsilon(x,y) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a(z) g_z^\varepsilon(x) \overline{g_z^\varepsilon}(y) dz$$

Denoting by κ_x the convolution kernel of $a \in \mathcal{S}(\mathbb{R}^{2d})$, we deduce that the convolution kernel of the operator $\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(a)$ is the function

$$\begin{aligned}\kappa_x^{\varepsilon,\mathrm{Wick}}(v) &:= (2\pi)^{-d} \int_{\mathbb{R}^{2d}} a(z) g_z^\varepsilon(x) \overline{g_z^\varepsilon}(x - \varepsilon v) dz \\ &= \pi^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{1}{2}|z - \sqrt{\varepsilon} v|^2 - \frac{1}{2}|z|^2} \kappa_{x - \sqrt{\varepsilon} z}(v) dz.\end{aligned}$$

Lemma 2.5. *Let $a \in \mathcal{S}(\mathbb{R}^{2d})$, there exists $C>0$ such that for all $\varepsilon \in (0,1]$,*

$$\|\mathrm{op}_\varepsilon^{\mathrm{Wick}}(a) - \mathrm{op}_\varepsilon^{\mathrm{KN}}(\sigma)\|_{\mathscr{L}(L^2(G))} \leq C\varepsilon.$$

Proof. We estimate the norms thank to the convolution kernels:

$$\begin{aligned}\|\mathrm{op}_\varepsilon^{\mathrm{KN}}(\sigma) - \mathrm{op}_\varepsilon^{\mathrm{Wick}}(\sigma)\|_{\mathscr{L}(L^2(G))} &\leq \int_{\mathbb{R}^d} \sup_{x\in\mathbb{R}^d} |\kappa_x^{\varepsilon,\mathrm{Wick}}(v) - \kappa_x(v)| dv \\ &\leq \pi^{-\frac{d}{2}} \int_{\mathbb{R}^d} \sup_{x\in\mathbb{R}^d} \left| \int_{\mathbb{R}^d} \mathrm{e}^{-\frac12|z|^2} \left(\mathrm{e}^{-\frac12|z-\sqrt{\varepsilon}v|^2} \kappa_{x-\sqrt{\varepsilon}z}(v) - \mathrm{e}^{-\frac12|z|^2}\kappa_x(v)\right) dz \right| dv.\end{aligned}$$

The result comes from a Taylor formula (in which the term in $\sqrt{\varepsilon}$ is equal to 0). □

2.2.3. *Gårding inequality and semiclassical measures.* The positivity of the Wick quantization implies the positivity of the Kohn-Niremberg quantization at leading order in the semi-classical limit.

Lemma 2.6. *Assume $a \geq 0$, then there exists a constant $C>0$ such that for all $f \in L^2(\mathbb{R}^d)$,*

$$(\mathrm{op}_\varepsilon^{\mathrm{KN}}(a) f, f)_{L^2} \geq -C\varepsilon \|f\|_{L^2}.$$

Theorem 2.7. *Let $(f^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$. There exists a sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ which tends to 0 when n goes to $+\infty$ and a positive measure μ on $\mathbb{R}^{2d}$ such that*

$$\forall a \in C_c^\infty(\mathbb{R}^{2d}),\ \left(\mathrm{op}_{\varepsilon_n}^{\mathrm{KN}}(a) f^{\varepsilon_n}, f^{\varepsilon_n}\right)_{L^2(\mathbb{R}^d)} \underset{n\to+\infty}{\longrightarrow} \int_{\mathbb{R}^{2d}} a(x,\xi)\mu(dx,d\xi). \tag{2.6}$$

Moreover $\mu(\mathbb{R}^{2d}) < +\infty$.

Any measure $\mu \in \mathcal{M}_+(\mathbb{R}^{2d})$ satisfying (2.6) for some sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ is called *Wigner measure* or *semi-classical measure* of the family $(f^\varepsilon)_{\varepsilon>0}$. A given family $(f^\varepsilon)_{\varepsilon>0}$ may have several Wigner measures.

Example 2.8. Let $x_0, \xi_0 \in \mathbb{R}^d$ and $\varphi \in L^2(\mathbb{R}^d)$.

1. *Concentration.* Let $u^\varepsilon(x) = \varepsilon^{-d/2}\varphi\left(\frac{\xi-\xi_0}{\varepsilon}\right)$, then $(u^\varepsilon)_{\varepsilon>0}$ has a unique Wigner measure
$$\mu_u(dx,d\xi) = (2\pi)^{-d}\,\delta_{x_0}(x) \otimes |\widehat{\varphi}(\xi)|^2 d\xi.$$
2. *Oscillation.* Let $v^\varepsilon(x) = \varphi(x)\mathrm{e}^{ix\cdot\xi_0/\varepsilon}$, then $(v^\varepsilon)_{\varepsilon>0}$ has a unique Wigner measure
$$\mu_v(dx,d\xi) = |\varphi(x)|^2 dx \otimes \delta_{\xi_0}(\xi).$$
3. *Gaussian wave packet.* The family $(g_z^\varepsilon)_{\varepsilon>0}$ defined in (1.2) has only one semi-classical measure which is the Dirac mass in z:
$$(\mathrm{op}_\varepsilon(a) g_z^\varepsilon, g_z^\varepsilon)_{L^2} \underset{\varepsilon\to0}{\longrightarrow} a(z).$$
4. *Coherent states.* Let $\varphi \in \mathcal{S}(\mathbb{R}^d)$ woth $\|\varphi\|_{L^2} = 1$, and $z=(q,p) \in \mathbb{R}^{2d}$. Then, the family
$$\mathrm{WP}_z^\varepsilon(\varphi) = \varepsilon^{-d/4}\varphi\left(\frac{x-q}{\sqrt{\varepsilon}}\right)\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)},,\quad x\in\mathbb{R}^d \tag{2.7}$$
also has only one the Dirac mass in z as semi-classical measure.

Proof. Since the quantity $I_\varepsilon(a) = (\mathrm{op}_\varepsilon(a) f^\varepsilon, f^\varepsilon)_{L^2(\mathbb{R}^d)}$ is uniformly bounded in ε, for a given function $a \in C_c^\infty(\mathbb{R}^{2d})$, one can find an extracted convergent subsequence $I_{\varepsilon_{n,a}}(a)$. Considering a dense countable subset of $C_c^\infty(\mathbb{R}^{2d})$ and using a diagonal extraction process, one builds a sequence ε_n for which $I_{\varepsilon_n}(a)$ has a limit for all $a \in C_c^\infty(\mathbb{R}^{2d})$ (see Appendix **??**). The map which sends a on the limit $I(a)$ of the sequence $I_{\varepsilon_n}(a)$ is a linear form on $C_c^\infty(\mathbb{R}^{2d})$. It defines a distribution and Gårding inequality shows that this distribution is positive.

It remains to prove that I satisfies a measure estimate. We consider a nonincreasing function $\chi \in C_c^\infty([0,+\infty))$ such that $0 \leq \chi \leq 1$, $\chi(u) = 0$ for $u \geq 2$ and $\chi(u) = 1$ for $0 \leq u \leq 1$. We set $\chi_R = \chi\left(\frac{\cdot}{R}\right)$ and consider $c_R = \chi_R(x)\chi_R(\xi)$. The convolution kernel associated with c_R is the function $k_R(x,v) = R^d\widehat{\chi}(Rv)\chi_R(x)$. Therefore, for all $R > 1$, we have

$$(\mathrm{op}_\varepsilon(c_R)f^\varepsilon, f^\varepsilon)_{L^2(\mathbb{R}^d)} \leq \|\widehat{\chi}\|_{L^1(\mathbb{R}^d)}.$$

Moreover, for $R \leq R'$, we have $c_R \leq c_{R'}$, whence $I(c_R) \leq I(c_{R'})$ and the sequence $I(c_R)$ converges. We call $I(1)$ its limit. Let $a \in C_c^\infty(\mathbb{R}^{2d})$. There exists $R_0 > 0$ such that for all $R > R_0$, $a = ac_R$. We deduce

$$0 = ac_R - a = a - \|a\|_{L^\infty}c_R + (\|a\|_{L^\infty} - a)c_R,$$

whence, using $(\|a\|_{L^\infty} - a)c_R \geq 0$ and the positivity of the distribution I,

$$0 \geq I(a - \|a\|_{L^\infty}c_R) = I(a) - \|a\|_{L^\infty}I(c_R).$$

Letting R go to $+\infty$ and arguing similarly with $-a$, we obtain the measure's type control that we were looking for:

$$I(a) \leq \|a\|_{L^\infty}I(1).$$

□

3. PROPAGATION OF COHERENT STATES AND THE QUANTUM-CLASSICAL CORRESPONDENCE

In this section, we study the properties of the coherent states defined in (2.7), namely

$$\mathrm{WP}^\varepsilon_z(\varphi) = \varepsilon^{-d/4}\varphi\left(\frac{x-q}{\sqrt{\varepsilon}}\right)\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)},\ \ x\in\mathbb{R}^d,$$

for $\varphi\in\mathcal{S}(\mathbb{R}^d)$ and $z\in\mathbb{R}^{2d}$. Note that, with the notation (1.2), we have for all $z\in\mathbb{R}^{2d}$,

$$g^\varepsilon_z = \mathrm{WP}^\varepsilon_z(g_0),\ \ g_0 = g^1_0.$$

The first important properties of coherent state is that it is a bounded family in $L^2(\mathbb{R}^d)$

$$\|\mathrm{WP}^\varepsilon_z(\varphi)\|_{L^2} = \|\varphi\|_{L^2},\ \ \forall\varphi\in\mathcal{S}(\mathbb{R}^d),\ \ \forall z\in\mathbb{R}^{2d}. \tag{3.1}$$

As we will see later, the coherent states enjoy localization properties that come from the simple way a pseudodifferential operator acts on them. This is particularly striking when one uses the Weyl quantization, which corresponds to the choice $t=\frac{1}{2}$ in (2.3). We use here the notation $\mathrm{op}_\varepsilon(a)$ for denoting the operator obtained by the Weyl quantization of the function $a\in\mathcal{S}(\mathbb{R}^d)$, and $\widehat{a}$ for the (non semiclassical) pseudodifferential operators, $\widehat{a}=\mathrm{op}_1(a)$.

In this section, we will first introduce functional spaces that are natural in this context. Then, we will study basic properties of the coherent states. Then, we will analyze their evolution through a family of Schrödinger equations.

3.1. **Weighted Sobolev spaces.** We introduce the functional spaces $\Sigma^k_\varepsilon := \Sigma^k_\varepsilon(\mathbb{R}^d)$ containing functions $f\in L^2(\mathbb{R}^d)$ such that

$$\forall\alpha,\beta\in\mathbb{N}^d,\ |\alpha|+|\beta|\le k,\ x^\alpha(\varepsilon\partial_x)^\beta f\in L^2(\mathbb{R}^d)$$

with a uniform control of the norm, with respect to $\varepsilon\in(0,1]$

$$\|f\|_{\Sigma^k_\varepsilon} = \sup_{|\alpha|+|\beta|\le k}\|x^\alpha(\varepsilon\partial_x)^\beta f\|_{L^2}.$$

For simplicity, we denote by Σ^k the sets Σ^k_ε corresponding to $\varepsilon=1$. The space Σ^k is a subspace of the Sobolev space $H^k(\mathbb{R}^d)$ and also of the vector space of functions whose Fourier transforms are in $H^k(\mathbb{R}^d)$. The space Σ^k_ε may then be understood as a semiclassical rescaled version of Σ^k. One has to notice that

$$\Sigma^0_\varepsilon = \Sigma^0 = L^2(\mathbb{R}^d)\ \text{ and }\ \mathcal{S}(\mathbb{R}^d) = \cap_{k\in\mathbb{N}}\Sigma^k.$$

Moreover, the coherent states belong to these spaces.

Lemma 3.1. *For all $k\in\mathbb{N}$, there exists $C_k>0$ such that for all $z_0=(q,p)\in\mathbb{R}^{2d}$ and $\varphi\in\mathcal{S}(\mathbb{R}^d)$,*

$$\|\mathrm{WP}^\varepsilon_{z_0}(\varphi)\|_{\Sigma^k_\varepsilon} \le C_k\sup_{\ell+p=k}\langle z_0\rangle^\ell\|\varphi\|_{\Sigma^p}.$$

Proof. Indeed, a straightforward calculus gives for $j\in\{1,\cdots d\}$

$$\begin{aligned}&x_j\mathrm{WP}^\varepsilon_{z_0}(\varphi) = \mathrm{WP}^\varepsilon_{z_0}((q_j+\sqrt{\varepsilon}y_j)\varphi),\\ &\varepsilon\partial_{x_j}\mathrm{WP}^\varepsilon_{z_0}(\varphi) = ip_j\mathrm{WP}^\varepsilon_{z_0}(\varphi)+\sqrt{\varepsilon}\mathrm{WP}^\varepsilon_{z_0}(\partial_{y_j}\varphi) = i\,\mathrm{WP}^\varepsilon_{z_0}((p_j+\sqrt{\varepsilon}D_{y_j})\varphi).\end{aligned}$$

We deduce that for $\alpha,\beta\in\mathbb{N}^d$,

$$x^\alpha(\frac{\varepsilon}{i}\partial_x)^\beta\mathrm{WP}^\varepsilon_{z_0}(\varphi) = \mathrm{WP}^\varepsilon_{z_0}((q+\sqrt{\varepsilon}y)^\alpha(p+\sqrt{\varepsilon}D_y)^\beta\varphi),$$

which allows to conclude by (3.1). $\square$

Let us now examine the action of semiclassical pseudodifferential operators in the spaces Σ_ε^k. For $1 \leq j \leq d$, the commutation relations between x_j or εD_{x_j} and $\mathrm{op}_\varepsilon(a)$ writes

$$[x_j, \mathrm{op}_\varepsilon(a)] = \varepsilon\, i\mathrm{op}_\varepsilon(\partial_{\xi_j} a) \text{ and } [\varepsilon D_{x_j}, \mathrm{op}_\varepsilon(a)] = -\varepsilon\, i\mathrm{op}_\varepsilon(\partial_{x_j} a). \tag{3.2}$$

Using these relations and the estimates in $L^2(\mathbb{R}^d)$, it is possible to prove estimates in Σ_ε^k that are uniform in ε. Let us denote by $N_d(a)$ a semi-norm such that for there exists a constant $C_d > 0$ such that for all $a \in \mathcal{S}(\mathbb{R}^d)$, one has

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C_d N_d(a).$$

Lemma 3.2. *Let $\varepsilon \in (0, 1]$ and $k \in \mathbb{N}$. There exist constants $C_{d,k}$ and c_k such that for all $a \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, we have in Σ_ε^k:*

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(\Sigma_\varepsilon^k)} \leq C_{d,k} \sup_{|\gamma| \leq k} N_d(\partial^\gamma a). \tag{3.3}$$

Proof. The proof is based on (3.2) and a recursive argument. For $a \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, $f \in \mathcal{S}(\mathbb{R}^d)$ and $j \in \{1, \cdots d\}$,

$$\|x_j \mathrm{op}_\varepsilon(a) f\|_{\Sigma_\varepsilon^{k-1}} \leq \|\mathrm{op}_\varepsilon(a)(x_j f)\|_{\Sigma_\varepsilon^{k-1}} + \varepsilon \|\mathrm{op}_\varepsilon(\partial_{\xi_j} a) f\|_{\Sigma_\varepsilon^{k-1}},$$
$$\|\varepsilon \partial_{x_j}(\mathrm{op}_\varepsilon(a) f)\|_{\Sigma_\varepsilon^{k-1}} \leq \|\mathrm{op}_\varepsilon(a)(\varepsilon \partial_{x_j} f)\|_{\Sigma_\varepsilon^{k-1}} + \varepsilon \|\mathrm{op}_\varepsilon(\partial_{x_j} a) f\|_{\Sigma_\varepsilon^{k-1}}.$$

Therefore, there exists a constant c' such that

$$\begin{aligned} \|\mathrm{op}_\varepsilon(a) f\|_{\Sigma_\varepsilon^k} \leq{}& c' \|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} \|f\|_{\Sigma_\varepsilon^k} \\ & + c' \sum_j \varepsilon \left(\|\mathrm{op}_\varepsilon(\partial_{\xi_j} a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} + \|\mathrm{op}_\varepsilon(\partial_{x_j} a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} \right) \|f\|_{\Sigma_\varepsilon^{k-1}}. \end{aligned}$$

One then concludes by starting the recursive argument from the boundedness of pseudodifferential operators in $\Sigma_\varepsilon^0 = L^2(\mathbb{R}^d)$. ☐

3.2. **First properties of coherent states.** Along the next sections of this chapter, we shall use properties of wave packets that we sum-up here.

Lemma 3.3. *if $f, g \in \mathcal{S}(\mathbb{R}^d)$ and $z, z' \in \mathbb{R}^{2d}$, then*

$$\langle \mathrm{WP}_z^\varepsilon(f), \mathrm{WP}_{z'}^\varepsilon(g) \rangle = \mathrm{e}^{\frac{i}{\varepsilon} p' \cdot (q - q')} W[f, g] \left(\frac{z' - z}{\sqrt{\varepsilon}} \right) \tag{3.4}$$

where the function $W[f, g]$ is the Schwartz function on $\mathbb{R}^{2d}$ defined by

$$W[f, g](\zeta) = \int_{\mathbb{R}^d} \overline{f}(x) g(x - q) \mathrm{e}^{ip \cdot x} dx, \;\; \zeta = (q, p).$$

Moreover, for all $n \in \mathbb{N}$, there exists a constant $C_n > 0$ such that

$$\forall \zeta \in \mathbb{R}^{2d}, \;\; \langle \zeta \rangle^n \, |W[f, g](\zeta)| \leq C_n \|f\|_{\Sigma^n} \|g\|_{\Sigma^n}. \tag{3.5}$$

Proof. The formula for $\langle \mathrm{WP}_z^\varepsilon(f), \mathrm{WP}_{z'}^\varepsilon(g) \rangle$ comes from a simple computation. Then, for $\alpha, \gamma \in \mathbb{N}^d$ and $z = (q, p) \in \mathbb{R}^{2d}$, we observe

$$\begin{aligned} |q^\gamma p^\alpha W[f, g](z)| &= \left| q^\gamma \int_{\mathbb{R}^d} D_x^\alpha (\overline{f}(x) g(x - q)) \mathrm{e}^{ix \cdot p} dx \right| \\ &\leq \langle q \rangle^{|\gamma|} \int_{\mathbb{R}^d} \left| D_x^\alpha (\overline{f}(x) g(x - q)) \right| dx \\ &\leq 2^{\frac{|\gamma|}{2}} \int_{\mathbb{R}^d} \langle x \rangle^{|\gamma|} \langle x - q \rangle^{|\gamma|} \left| D_x^\alpha (\overline{f}(x) g(x - q)) \right| dx \end{aligned}$$

where we have used Peetre inequality

$$\forall t \in \mathbb{R},\ \ \forall \ell \in \mathbf{Z},\ \ \frac{\langle t\rangle^{\ell}}{\langle t'\rangle^{\ell}} \leq 2^{\frac{|\ell|}{2}} \langle t-t'\rangle^{|\ell|}. \tag{3.6}$$

The conclusion then follows. ☐

3.3. **Coherent states and pseudodifferential operators.** The coherent states enjoy localization properties that come from the simple way a pseudodifferential operator acts on them. This is particularly striking when one uses the Weyl quantization, which corresponds to the choice $t=\frac{1}{2}$ in (2.3). We use here the notation $\mathrm{op}_\varepsilon(a)$ for denoting the operator $\mathrm{op}_\varepsilon^{\frac{1}{2}}(a)$ obtained by the Weyl quantization of the function $a \in \mathcal{S}(\mathbb{R}^d)$, and $\widehat{a}$ for the (non semiclassical) pseudodifferential operators, $\widehat{a} = \mathrm{op}_1(a)$.

Lemma 3.4. *Let $z_0=(q,p)\in\mathbb{R}^{2d}$, $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$. Then,*

$$\mathrm{op}_\varepsilon(a)\,\mathrm{WP}^\varepsilon_{z_0}(\varphi) = \mathrm{WP}^\varepsilon_{z_0}\left(\widehat{a(z_0+\sqrt{\varepsilon}z)}\,\varphi\right).$$

Proof. The result comes from a simple change of variables. One writes

$$\begin{aligned}\mathrm{op}_\varepsilon(a)\,\mathrm{WP}^\varepsilon_{z_0}(\varphi)(x) &= (2\pi\varepsilon)^{-d}\varepsilon^{-d/4}\int a\left(\frac{x+x'}{2},\xi\right)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-x')+\frac{i}{\varepsilon}p\cdot(x'-q)}\varphi\left(\frac{x'-q}{\sqrt{\varepsilon}}\right)dx'd\xi\\ &= (2\pi\varepsilon)^{-d}\varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\int a\left(\frac{x+x'}{2},\xi\right)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-x')-\frac{i}{\varepsilon}p\cdot(x-x')}\varphi\left(\frac{x'-q}{\sqrt{\varepsilon}}\right)dx'd\xi.\end{aligned}$$

Then the change of variables $x'=q+\sqrt{\varepsilon}\,y'$ and $\xi = p+\sqrt{\varepsilon}\eta$ gives

$$\begin{aligned}\mathrm{op}_\varepsilon(a)\,\mathrm{WP}^\varepsilon_{z_0}(\varphi)(x) &= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\left((2\pi)^{-d}\int a\left(\frac{x+q+\sqrt{\varepsilon}y'}{2},p+\sqrt{\varepsilon}\eta\right)\mathrm{e}^{i\eta\cdot\left(\frac{(x-q)}{\sqrt{\varepsilon}}-y'\right)}\varphi(y')dy'd\eta\right)\\ &= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\Phi^\varepsilon\left(\frac{x-q}{\sqrt{\varepsilon}}\right)\\ &= \mathrm{WP}^\varepsilon_{z_0}(\Phi^\varepsilon)(x),\end{aligned}$$

with

$$\Phi^\varepsilon(y) = (2\pi)^{-d}\int a\left(q+\sqrt{\varepsilon}\frac{y+y'}{2},\xi\right)\mathrm{e}^{i(p+\sqrt{\varepsilon}\eta)\cdot(y-y')}\varphi(y')dy'd\eta = \widehat{a(z_0+\sqrt{\varepsilon}z)}\,\varphi,$$

which terminates the proof. ☐

Lemma 3.4 has two several important consequences that are stated below. First, one can say that a coherent state only sees the action of a semiclassical pseudodifferential operator through the Taylor series of the symbol of the pseudo at the core of the coherent state.

Lemma 3.5. *Let $\varepsilon\in(0,1]$, $z_0=(q,p)\in\mathbb{R}^{2d}$, $\varphi\in\mathcal{S}(\mathbb{R}^d)$ and $a\in\mathcal{C}^\infty(\mathbb{R}^{2d})$ bounded together with its derivatives. Then, we have the following properties: For all $n,k\in\mathbb{N}$, there exists a constant $C_{k,n}$ such that*

$$\left\|\mathrm{op}_\varepsilon(a)\,\mathrm{WP}^\varepsilon_{z_0}(\varphi) - \mathrm{WP}^\varepsilon_{z_0}\left(\widehat{P_a^{(n_0)}(z\sqrt{\varepsilon})}\varphi\right)\right\|_{\Sigma^k_\varepsilon} \leq C_{k,n}\,\varepsilon^{\frac{n+1}{2}}\left(\sup_{|\gamma|\leq k+n+1} N_d(\partial^\gamma a)\right)\|\varphi\|_{\Sigma^{k+n+1}}$$

where $z\mapsto P_a^{(n)}(z)$ is the Taylor polynomial at order n_0 of a in z_0:

$$P_a^{(n_0)}(z) = a(z_0)+\nabla a(z_0)\cdot z + \frac{1}{2}\nabla^2 a(z_0)z\cdot z + \ldots + \frac{1}{n!}d^n a(z_0)[z]^n.$$

As a consequence, since for a function identically equal to 1 close to z_0, its Taylor polynomial is the constant 1 at any order, a coherent state is highly localized microlocally close to its core, in a sense that the next statement makes precise.

Corollary 3.6. Microlocalisation of coherent states. *Moreover, assume that* $a(z) = 1$ *for* $|z-z_0| \leq 1$ *and* $a(z) = 0$ *if* $|z - z_0| > 2$. *Then, for any* $n \in \mathbb{N}$, *there exists a constant* $C'_{k,n}$ *such that*

$$\|\mathrm{WP}^{\varepsilon}_{z_0}(\varphi) - \mathrm{op}_{\varepsilon}(a)\,\mathrm{WP}^{\varepsilon}_{z}(\varphi)\|_{\Sigma^k_{\varepsilon}} \leq C'_{k,n}\,\varepsilon^{n/2} \left(\sup_{|\gamma| \leq k+n} N_d(\partial^{\gamma} a) \right) \|\varphi\|_{\Sigma^{k+n}}.$$

Proof of Lemma 3.5. Let us prove Point (1). Applying Lemma 3.4,

$$\|\mathrm{op}_{\varepsilon}(a)\,\mathrm{WP}^{\varepsilon}_{z_0}(\varphi) - \mathrm{WP}^{\varepsilon}_{z_0}(\widehat{P_a^{(n)}(z\sqrt{\varepsilon})}\varphi)\|_{\Sigma^k_{\varepsilon}} = \|\mathrm{WP}^{\varepsilon}_{z_0}((\widehat{a(z_0 + \sqrt{\varepsilon}z)} - \widehat{P_a^{(n)}(z\sqrt{\varepsilon})})\varphi)\|_{\Sigma^k_{\varepsilon}}.$$

By Lemma 3.1, there exists a constant C_k such that for all profiles $\varphi \in \mathcal{S}(\mathbb{R}^d)$,

$$\|\mathrm{WP}^{\varepsilon}_{z_0}(\varphi)\|_{\Sigma^k_{\varepsilon}} \leq C_k \|\varphi\|_{\Sigma^k}$$

hence

$$\|\mathrm{WP}^{\varepsilon}_{z_0}((\widehat{a(z_0 + \sqrt{\varepsilon}z)} - \widehat{P_a^{(n)}(z\sqrt{\varepsilon})})\varphi)\|_{\Sigma^k_{\varepsilon}} \leq C'_k \|(\widehat{a(z_0 + \sqrt{\varepsilon}z)} - \widehat{P_a^{(n)}(z\sqrt{\varepsilon})})\varphi\|_{\Sigma^k}.$$

Moreover, we have

$$a(z_0 + \sqrt{\varepsilon}z) - P_a^{(n)}(z\sqrt{\varepsilon}) = \varepsilon^{\frac{n+1}{2}} r(\sqrt{\varepsilon}z)[z]^{n+1}$$

where $r \in \mathcal{C}^{\infty}(\mathbb{R}^{2d})$ is a smooth tensor of order $n+1$ that is bounded with bounded derivatives

$$r(z) = \frac{1}{n!} \int_0^1 d^{(n+1)} a(z_0 + sz)(1-s)^n ds.$$

The result then comes from the existence of a constant $c_{k,n}$ such that for all $\gamma \in \mathbb{N}^{2d}$,

$$\|\mathrm{op}_1(r(\sqrt{\varepsilon}z)z^{\gamma})\varphi\|_{\Sigma^k} \leq c_{k,n} \|\varphi\|_{\Sigma^{k+|\gamma|}} \sup_{|\gamma| \leq n+k+1} N_d(r). \tag{3.7}$$

The property (3.7) is obvious when $|\gamma| = 0$. In the general case, one obtains it by a recursive process based on the commutation relations (3.2). □

4. The quantum classical correspondence

4.1. **Euristics.**

Consider a semiclassical evolution equation of pseudodifferential type

$$i\varepsilon\partial_t\psi^\varepsilon = \mathrm{op}_\varepsilon(H)\psi^\varepsilon. \tag{4.1}$$

Let us assume that the function $H = H(x,\xi)$ satisfies adequate properties so that there exists a solution once fixed an initial data. We focus on initial data of the form

$$\psi^\varepsilon_{|t=0} = \mathrm{WP}^\varepsilon_z(\varphi),\ \ \varphi\in\mathcal{S}(\mathbb{R}^d),\ \ z=(q,p),$$

and we look for solutions of the same form,

$$\psi^\varepsilon(t,\cdot) = \mathrm{WP}^\varepsilon_{z(t)}(b^\varepsilon(t,\cdot)),$$

for some adequate time-dependent core function $z(t) = (q(t),p(t))$ and time-dependent profile $b^\varepsilon(t,\cdot)$, that we aim at determining. A simple computation gives

$$\begin{aligned}(\mathrm{WP}^\varepsilon_{z(t)})^{-1}(i\varepsilon\partial_t - \mathrm{op}_\varepsilon(H))\mathrm{WP}^\varepsilon_{z(t)} &= p(t)\cdot\dot q(t) - H(q(t),p(t))\\ &\quad+\sqrt{\varepsilon}\left(\dot q(t)\cdot D_y - \dot p(t)\cdot y - \nabla H(q(t),p(t))\cdot {}^t(y,D_y)\right)\\ &\quad+\varepsilon\left(i\partial_t - \frac{1}{2}\mathrm{Hess}H(q(t),p(t)(y,D_y)\cdot(y,D_y)\right) + O(\varepsilon^{\frac{3}{2}}).\end{aligned}$$

As a consequence, it is natural to choose the function $b^\varepsilon(t,x)$ of the form

$$b^\varepsilon(t,x) = \mathrm{e}^{\frac{i}{\varepsilon}S(t)}u^\varepsilon(t,x)$$

with

$$\dot S(t) = p(t)\cdot\dot q(t) - H(q(t),p(t)),\ \ S(0)=0, \tag{4.2}$$

and u^ε solution to the equation

$$\begin{cases} i\partial_t u^\varepsilon(t,y) = \frac{1}{2}\mathrm{Hess}H(q(t),p(t))(y,D_y)\cdot(y,D_y)u^\varepsilon(t,y), & (t,y)\in\mathbb{R}\times\mathbb{R}^d\\ u^\varepsilon_{|t=0} = \varphi, \end{cases}$$

and the time-dependent core $z(t) = (q(t),p(t))$ such that

$$\begin{cases} \dot q(t) = \nabla_\xi H(q(t),p(t)), & q(0)=q,\\ \dot p(t) = \nabla_x iH(q(t),p(t)), & p(0)=p. \end{cases}$$

The curves $(q(t),p(t))$ are the *classical trajectories* associated with the Hamiltonian function $H(x,\xi)$ in the framework of classical mechanics. They satisfy

$$H(q(t),p(t)) = H(q,p),\ \ \forall t\in\mathbb{R}.$$

One also talks of the *Hamiltonian curves* of the function H. The function $S(t)$ is called the *classical action*. Thus, the wave packet approximation of the solutions of the evolution equation (4.1) that we have sketched here connects the quantum evolution $\psi^\varepsilon(t,x)$ with classical quantities reminiscent of the classical mechanics. One talks of the *quantum classical correspondence* that holds in the *semiclassical regime*, $\varepsilon\to 0$. The objective of the next section is to make these Euristics rigorous.

4.2. **The classical trajectories.**

We consider the hamiltonian

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

and assume that the potential V is smooth and at most quadratic:

$$\forall\alpha\in\mathbb{N}^d,\ \ |\alpha|\geq 2,\ \ \exists C_\alpha>0,\ \ \|\partial^\alpha V\|_{L^\infty}\leq C_\alpha. \tag{4.3}$$

The equation of the classical trajectories write

$$\dot q = p\ \text{ and }\ \dot p = -\nabla V(q)$$

and the action is given by

$$S(t)=\int_0^t\left(\frac{|p(s)|^2}{2}-V(q(s))\right)ds,\ \ t\in\mathbb{R}.$$

One recognizes the Newtonian equation $\ddot q=-\nabla V(q)$. Because of the assumption on the potential V, these trajectories are globally defined and grow at most exponentially (see for example the book [3]).

Lemma 4.1. Classical trajectories. *Assume V satisfies the assumption* (4.3)*, then there exist $C_0, C_1>0$ such that*

$$|q(t)|+|p(t)|\leq C_0\mathrm{e}^{C_1|t|},\ \ \forall t\in\mathbb{R}.$$

Proof. The existence for all times comes from Cauchy-Lipschitz Theorem. Indeed, the function $z(t)=(q(t),p(t))$ satisfies for all $t\in\mathbb{R}$, $\dot z(t)=\nabla H(z(t))$ with $z\mapsto\nabla H(t)$ being Lipchitz by (4.3). Indeed, it implies $|\nabla V(x)|\leq c(1+|x|)$ for some constant $c>0$. Combined with the relation $H(q(t),p(t))=H(q,p)$, it also implies the existence of $C>0$ such that

$$|p(t)|=|\dot q(t)|\leq C(1+|q(t)|),\ \ \forall t\in\mathbb{R},$$

and the estimate follows by Grönwall's lemma. □

4.3. **The profile equation.** Let us now examine the profile equation which is a Schrödinger equation with a time-dependent quadratic potential

$$\left\{\begin{array}{l} i\partial_t u(t,y)=\frac12\Delta_y u(t,y)+\frac12\mathrm{Hess}V(q(t))y\cdot yu(t,y),\ \ (t,y)\in\mathbb{R}\times\mathbb{R}^d\\ u_{|t=0}=\varphi.\end{array}\right.\tag{4.4}$$

Under the assumption (4.3) on the growth of the potential V, there exist solutions to (B.1) (see Remark 4.3 below). Moreover, one can also prove that this solution is Schwartz, with a control of its semi-norms that is exponentially large in time.

Lemma 4.2. *For all $k\in\mathbb{N}$, there exists constants c_k and C_k such that for all $\varphi\in\Sigma^k$, the solution of equation* (B.1) *satisfies*

$$\|u(t,\cdot)\|_{\Sigma^k}\leq C_k\mathrm{e}^{c_k|t|}\|\varphi\|_{\Sigma^k},\ \ \forall t\in\mathbb{R}.$$

Proof. The proof relies in a recursive argument in $k\in\mathbb{N}$, starting with $k=0$ and writing a closed system on $y^\alpha\partial_y^\beta u(t,\cdot)$ for all $\alpha,\beta\in\mathbb{N}^d$ such that $|\alpha|+|\beta|=k$. □

The estimates of these two Lemma are sharp, as shown by the quadratic potential $V(x)=\frac{|x|^2}{2}$ shows it. Indeed, there exists the Hilbertian basis $(f_n)_{n\in\mathbb{N}}$ of the Hermite functions, satisfy

$$(-\frac12\Delta+\frac{|x|^2}{2})f_n=\lambda_n f_n,\ \ 0<\lambda_n\underset{n\to+\infty}{\longrightarrow}+\infty.$$

Therefore, starting with $\varphi=f_n$, $u(t,.)=\mathrm{e}^{t\lambda_n}$ has exactly exponential growth.

Lemma 4.2 implies the existence of a semi-group $\mathcal{U}(t,s)$, a two parameters family of unitary operators of $L^2(\mathbb{R}^d)$, such that for all $(t,s)\in\mathbb{R}$,

$$\left\{\begin{array}{l} i\partial_t\mathcal{U}(t,s)=\left(\frac12\Delta_y+\frac12\mathrm{Hess}V(q(t))y\cdot y\right)\mathcal{U}(t,s),\\ \mathcal{U}(s,s)=\mathrm{Id}_{L^2(\mathbb{R}^d)}.\end{array}\right.\tag{4.5}$$

These propagators act continuously on the spaces Σ^k for all $k\in\mathbb{N}$.

Remark 4.3. In the exercices of the Appendix, are treated the following points:
(i) If $\varphi(y) = \pi^{-\frac{d}{4}} \mathrm{e}^{-\frac{|y|^2}{2}}$ for $y \in \mathbb{R}^d$, then it is proved in [2] that $u(t, y)$ is given by an explicit formula. Define $F(t, z_0) = \partial_z \Phi^t(z_0) \in \mathbb{R}^{2d}$ where $\Phi^t(z_0)$ is the flow map,

$$\Phi^t(z_0) = {}^t(q(t), p(t)).$$

Then F solves the system

$$\partial_t F(t, z_0) = \begin{pmatrix} 0 & \mathrm{Id}_{\mathbb{R}^d} \\ -\mathrm{Hess}V(q(t)) & 0 \end{pmatrix}, \quad F(0, z_0) = \mathrm{Id}_{\mathbb{R}^{2d}}.$$

We set

$$F(t, z_0) = \begin{pmatrix} A(t, z_0) & B(t, z_0) \\ C(t, z_0) & D(t, z_0) \end{pmatrix} \tag{4.6}$$

and we have

$$\begin{aligned} &u(t, y) = c_{\Gamma(t,z_0)} \mathrm{e}^{i\Gamma(t,z_0)y\cdot y}, \quad y \in \mathbb{R}^d, \\ &\Gamma(t, z_0) = (C(t, z_0) + iD(t, z_0))(A(t, z_0) + iB(t, z_0))^{-1}, \\ &c_{\Gamma(t,z_0)} = \pi^{-\frac{d}{4}} \det{}^{-1/2}(A(t, z_0) + iB(t, z_0). \end{aligned}$$

(ii) More generally, one can construct a Hermitian basis of explicit solutions to the equation, with similarities with the Hermite functions. These functions were constructed by George Hagedorn (see [9]), the construction is also explained in [19] (see section 3).

The construction of this semi-group allows to solve profile equations with source terms $f(t, \cdot)$ that are smooth functions in t valued in the set of Schwartz functions.

$$\left\{ \begin{array}{l} i\partial_t u(t, y) = -\frac{1}{2}\Delta_y u(t, y) + \frac{1}{2}\mathrm{Hess}V(q(t))y \cdot yu(t, y) + f(t, y), \quad (t, y) \in \mathbb{R} \times \mathbb{R}^d \\ u_{|t=0} = \varphi. \end{array} \right. \tag{4.7}$$

Indeed, the solution is then given by the Duhamel formula

$$u(t, \cdot) = \mathcal{U}(t, 0)\varphi + \frac{1}{i}\int_0^t \mathcal{U}(t, s) f(s, \cdot) ds,$$

and it is a Schwartz function if φ and $f(t, \cdot)$ are such for all $t \in \mathbb{R}$. All these elements allow to conclude about the form of the solution of the Schrödinger equation for initial data that are coherent states.

An additional property of this semigroup consists in its action on pseudodifferential operators

Lemma 4.4. *Let $a \in \mathcal{S}(\mathbb{R}^{2d})$, then for all $s, t \in \mathbb{R}$,*

$$\mathcal{U}(t, s)\mathrm{op}_1^w(a)\mathcal{U}(t, s) = \mathrm{op}_1^w(a \circ \Psi^{s,t}).$$

where $\Psi^{t,s}(y, \eta) = (x^{t,s}(y, \eta), \xi^{t,s}(y, \eta)$ is the flow map defined by the trajectories

$$\frac{d}{dt}x^{t,s}(y, \eta) = \xi^{t,s}(y, \eta), \quad \frac{d}{dt}\xi^{t,s}(y, \eta) = -V''(q(t))x^{t,s}(y, \eta) \text{ and } x^{t,t}(y, \eta) = y, \quad \xi^{t,t}(y, \eta) = \eta.$$

Moreover, the map $(y, \eta) \mapsto \Psi{\cdot}t, s(y, \eta) = (x^{t,s}(y, \eta), \xi^{t,s}(y, \eta)$ is linear

Such a result is called a Egorov Theorem. It holds for non quadratic Hamiltonian with a semiclassical quantization and then hods up to a remainder. What is specific to the quadratic Hamiltonian is the absence of rest term.

Proof. Let $s, t \in \mathbb{R}$, $s \le t$, $\sigma \in [s,t]$ and $b(\sigma, \cdots) \in \mathcal{S}(\mathbb{R}^{2d})$ be defined for $\sigma \in [s,t]$ by

$$b(\sigma, x^{t,\sigma}(y,\eta), \xi^{t,\sigma}(y,\eta)) = a(y,\eta).$$

We then have for all $y, \eta \in \mathbb{R}^d$ and $\sigma \in [s,t]$,

$$\partial_\sigma b(\sigma, y, \eta) + \eta \cdot \nabla_y b(\sigma, y, \eta) - V''(q(t)) y \cdot \nabla_\eta b(\sigma, y, \eta) = 0.$$

We deduce from symbolic calculus

$$\frac{d}{d\sigma}\left(\mathcal{U}(\sigma,s)^* \mathrm{op}_1^w(b(\sigma)) \mathcal{U}(\sigma,s)\right) = 0,$$

which implies

$$\mathcal{U}(t,s)^* \mathrm{op}_1^w(b(t)) \mathcal{U}(t,s) = \mathrm{op}_1^w(b(s))$$

or equivalently

$$\mathcal{U}(t,s) \mathrm{op}_1^w(a) \mathcal{U}(t,s) = \mathrm{op}_1^w(a \circ \Psi^{s,t}).$$

The linearity of the flow map comes from the analysis of the ODE satisfied by $t \mapsto \nabla_z \Phi^{t,s}(z)$. $\square$

4.4. **Wave packets propagation by the Schrödinger propagator.** We can now state the approximation result. With $\varphi \in \mathcal{S}(\mathbb{R})$, we associate the approximate solution

$$\psi^\varepsilon_{\mathrm{app}}(t,x) = \mathrm{e}^{\frac{i}{\varepsilon} S(t)} \mathrm{WP}^\varepsilon_{z(t)}(u(t,\cdot)(x), \quad x \in \mathbb{R}^d,$$

where $u(t,\cdot)$ is the unique solution of (B.1).

Theorem 4.5. *For all $k \in \mathbb{N}$, there exists two constants $C_k, c_k > 0$ such that satisfies*

$$\| \psi^\varepsilon(t,\cdot) - \psi^\varepsilon_{\mathrm{app}}(t,\cdot) \|_{\Sigma^k} \le \sqrt{\varepsilon}\, C_k \mathrm{e}^{c_k |t|} \|\varphi\|_{\Sigma^3}, \quad t \in \mathbb{R}.$$

Proof. For $k = 0$, the proof relies on an energy estimate. Indeed, by construction, the function $w^\varepsilon = \psi^\varepsilon - \psi^\varepsilon_{\mathrm{app}}$ satisfies $w^\varepsilon(0,\cdot) = 0$ and

$$i\varepsilon \partial_t w^\varepsilon(t,x) + \frac{\varepsilon^2}{2} \Delta w^\varepsilon(t,x) - V(x) w^\varepsilon(t,x) = \varepsilon^{\frac{3}{2}} \mathrm{WP}^\varepsilon_{z(t)} \left(\int_0^1 V^{(3)}(q(t) + \tau \sqrt{\varepsilon} y)[y]^3 (1-\tau)^2 u(t,y) d\tau \right).$$

This implies

$$\| w^\varepsilon(t) \|_{L^2} \le \sqrt{\varepsilon} \| V^3 \|_{L^\infty} \| u(t,\cdot) \|_{\Sigma^3}.$$

The case $k \neq 0$ comes from a recursive argument. $\square$

One can prove a more precise statement and show that $\psi^\varepsilon(t)$ is asymptotic at any order in ε to a superposition of wave packets.

Theorem 4.6. *There exists a sequence of time-dependent Schwartz functions $(u_j(t,\cdot))_{j \ge 0}$ depending smoothly in t such that $u_0 = u$*

$$\psi^\varepsilon(t,x) = \mathrm{e}^{\frac{i}{\varepsilon} S(t)} \left(\sum_{j=0}^n \varepsilon^{\frac{j}{2}} \mathrm{WP}^\varepsilon_{z(t)}(u_j(t,\cdot))(x) + \varepsilon^{\frac{n+1}{2}} \mathrm{WP}^\varepsilon_{z(t)}(w^\varepsilon(t,\cdot))(x) \right), \quad (t,x) \in \mathbb{R} \times \mathbb{R}^d,$$

with for all $k, n \in \mathbb{N}$, there exists two constants $C_{k,n}, c_{k,n} > 0$ such that

$$\| w^\varepsilon(t,\cdot) \|_{\Sigma^k} \le \varepsilon^{\frac{n+1}{2}} C_{k,n}, \quad t \in \mathbb{R}.$$

Proof. One works on the function $u^\varepsilon(t)$ such that

$$\mathrm{WP}^\varepsilon_{z(t)}(u^\varepsilon(t,\cdot)) = \psi^\varepsilon(t,\cdot).$$

This function satisfies

$$i\partial_t u^\varepsilon = -\frac{1}{2}\Delta u^\varepsilon + \mathcal{V}^\varepsilon(t,y)u^\varepsilon(t,y), \;\; u^\varepsilon_{|t=0} = \varphi,$$

with

$$\mathcal{V}^\varepsilon(t,y) = \frac{1}{\varepsilon}(V(q(t)+\sqrt{\varepsilon}y) - V(q(t)) - \sqrt{\varepsilon}V'(q(t))y).$$

Let $n \in \mathbb{N}$. Consider $u_0, \cdots, u_n$ such that

$$i\partial_t u_0 = -\frac{1}{2}\Delta u_0 + \frac{1}{2}V''(q(t))[y]^2 u_0, \;\; u_0(0,\cdot) = \varphi,$$

and, for $j \geq 1$

$$i\partial_t u_j = -\frac{1}{2}\Delta u_j + \frac{1}{2}V''(q(t))[y]^2 u_j + \sum_{\ell=0}^{j-1} \frac{1}{(j-\ell+2)!} V^{(j-\ell+2)}(q(t))[y]^{j-\ell+2}u_\ell, \;\; u_j(0,\cdot) = 0.$$

Then the function

$$w^\varepsilon = u^\varepsilon - u_0 - \sqrt{\varepsilon}u_1 - \cdots - \varepsilon^{\frac{n}{2}}u_n$$

satisfies

$$i\partial_t w^\varepsilon(t,y) = -\frac{1}{2}\Delta w^\varepsilon(t,y) + \mathcal{V}^\varepsilon(t,y)w^\varepsilon(t,y) + f^\varepsilon(t,y), \;\; w^\varepsilon(0,\cdot) = 0,$$

$$f^\varepsilon(t,y) = \sum_{j=0}^{n} \varepsilon^{\frac{j}{2}} \left(\mathcal{V}^\varepsilon(t,y) - \sum_{k=2}^{n-j} \varepsilon^{\frac{k}{2}} \frac{1}{k!} V^{(k)}(q(t))[y]^k \right) u_j(t,y) = O(\varepsilon^{\frac{n+1}{2}}) \;\; in \;\; L^2(\mathbb{R}^d).$$

An energy identity implies $\|w(t,\cdot)\|_{L^2} = O(\varepsilon^{\frac{n+1}{2}})$. More generally, $\|w(t,\cdot)\|_{\Sigma^k_\varepsilon} = O(\varepsilon^{\frac{n+1}{2}})$ for all $k \in \mathbb{N}$. ☐

Remark 4.7. Note that if $\varphi = g_0$, the normalized centered Gaussian, then by Remark 4.3,

$$u_0(t,y) = c_{\Gamma(t,z_0)} \mathrm{e}^{i\Gamma(t,z_0)y\cdot y} =: g^{\Gamma(t,0)}(y), \;\; \forall y \in \mathbb{R}^d,$$

and $u_1(t,\cdot)$ satisfies

$$i\partial_t u_1(t,y) = -\frac{1}{2}\Delta u_1(t,y) + \frac{1}{2}V''(q(t))[y]^2 u_1(t,y) + \frac{1}{6}V^{(3)}q(t))[y]^3 g^{\Gamma(t,0)}(y), \;\; u_j(0,\cdot) = 0.$$

Therefore Duhamel's formula yields

$$u_1(t,y) = \frac{1}{6i}\int_0^t \mathcal{U}(t,s)V^{(3)}q(s))[y]^3 g^{\Gamma(s,0)}(y)ds.$$

Using Lemma 4.4, we deduce that there exists functions $b_\alpha(t)$ such that

$$u_1(t,y) = \sum_{|\alpha|=3} b_\alpha(t) y^\alpha g^{\Gamma(t,0)}(y), \;\; t \in \mathbb{R}, \;\; y \in \mathbb{R}^d.$$

4.5. **Additional properties.** The action defined in (4.2) depends on the initial point of the flow map

$$\Phi^t(z) = (\Phi_q^t(t,z), \Phi_p^t(t,z), \quad z = (q,p).$$

More precisely, we have for all $t \in \mathbb{R}$

$$\nabla_q S(t,z) = -p + A(t,z)\Phi_p^t(z) \ \text{ and } \ \nabla_p S(t,z) = B(t,z)\Phi_p^t(z), \quad z = (q,p)$$

where the matrices $A(t,z)$ and $B(t,z)$ are defined by (B.5):

$$A(t,z) = \partial_q \Phi_q^t(z) \ \text{ and } \ B(t,z) = \partial_p \Phi_q^t(z).$$

Proof. We have

$$\begin{aligned}\partial_q \dot{S}(t,z) &= \partial_q \Phi_p^t(z)\Phi_p^t(z) - \nabla_q \Phi_q^t(z)\nabla V(\Phi_q^t(z),\\ \partial_p \dot{S}(t,z) &= \partial_p \Phi_p^t(z)\Phi_p^t(z) - \nabla_p \Phi_q^t(z)\nabla V(\Phi_q^t(z)\end{aligned}$$

We verify the two relations by differentiation in t and observing

$$\begin{aligned}&\nabla_q S(0,z) = 0, \ \ A(0,z) = \mathrm{Id}, \ \ \Phi_p^0(z) = p,\\ &\nabla_p S(0,z) = 0, \ \ B(0,z) = 0.\end{aligned}$$

We verify

$$\begin{aligned}&\frac{d}{dt}(\nabla_q S(t,z) + p - A(t,z)\Phi_p^t(z)) = \partial_q \dot{S}(t,z) - \partial_q \dot{\Phi}_q^t(z)\Phi_p^t(z) - \partial_q \Phi_q^t(z)\dot{\Phi}_p^t(z)\\ &\quad = \partial_q \Phi_p^t(z)\Phi_p^t(z) - \nabla_q \Phi_q^t(z)\nabla V(\Phi_q^t(z) - \nabla_q \Phi_p^t(z)\Phi_p^t(z) + \nabla_q \Phi_q^t(z)\nabla V(\Phi_q^t(z)) = 0,\\ &\frac{d}{dt}(\nabla_p S(t,z) - B(t,z)\Phi_p^t(z)) = \nabla_p \dot{S}(t,z) - \nabla_p \dot{\Phi}_q^t(z)\Phi_p^t(z) - \nabla_p \Phi_q^t(z)\dot{\Phi}_p^t(z)\\ &\quad = \partial_p \Phi_p^t(z)\Phi_p^t(z) - \nabla_p \Phi_q^t(z)\nabla V(\Phi_q^t(z)) - \partial_p \Phi_p^t(z)\Phi_p^t(z) + \nabla_p \Phi_q^t(z)\nabla V(\Phi_q^t(z)) = 0.\end{aligned}$$

$\square$

5. HERMAN-KLUK PROPAGATOR

In this section, we construct approximations of the propagator associated with the semiclassical Schrödinger operator

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

In other words we are looking for an approximation formula of the solution $\psi^\varepsilon(t)$ of the equation

$$\tag{5.1} \left\{ \begin{array}{l} i\varepsilon\partial_t\psi^\varepsilon(t,x) = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon(t,x) + V(x)\psi^\varepsilon(t,x), \ \ (t,x)\in\mathbb{R}\times\mathbb{R}^d \\ \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0, \end{array}\right.$$

for initial data that are bounded in $L^2(\mathbb{R}^d)$. These approximations are based on the use of Bargmann transform. Therefore, we first focus on the properties of the class of operators we want to consider. Then, we will present two sorts of representations, the *thawed Gaussian approximation*, and the *frozen Gaussian approximation*, which is also referred to as *Herman-Kluk propagator* in the literature. These approximations combine the frame property of the set of Gaussian wave packets (2.5), and the description of section 4.4 of the action on Gaussians wave packets of the semiclassical Schrödinger propagator.

5.1. **Bargmann multipliers.** In this section, we introduce a class of operators constructed via the Bargmann transform. Consider a smooth family of the form

$$(z\mapsto\theta^\varepsilon_z)\in\mathcal{C}^\infty(\mathbb{R}^{2d}_z, L^2(\mathbb{R}^d)).$$

We call *Bargmann multiplier* associated with this family and we denote by $\mathcal{J}[\theta^\varepsilon_z]$ the operator acting on $\phi\in L^2(\mathbb{R}^d)$ according to

$$\tag{5.2} \mathcal{J}[\theta^\varepsilon_z](\phi)(x) = (2\pi\varepsilon)^{-\frac{d}{2}}\int_{\mathbb{R}^{2d}}\mathcal{B}^\varepsilon[\phi](z)\theta^\varepsilon_z(x)dz = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}\langle g^\varepsilon_z,\phi\rangle\theta^\varepsilon_z(x)dz, \ \ x\in\mathbb{R}^d.$$

The Gaussian frame identity (2.5) also writes with these notations

$$\mathcal{J}[g^\varepsilon_z] = \mathrm{Id}_{L^2(\mathbb{R}^d)}.$$

Indeed, $\mathcal{J}[g^\varepsilon_z]$ is obtained by composition of the operator of multiplication by θ^ε_z by the Bargmnna transform and its adjoint

$$\mathcal{J}[g^\varepsilon_z] = (\mathcal{B}^\varepsilon)^*\circ\theta^\varepsilon_z\circ\mathcal{B}^\varepsilon.$$

The formal adjoint of $\mathcal{J}[\theta^\varepsilon_z]$ is

$$\tag{5.3} \mathcal{J}[\theta^\varepsilon_z]^* : \phi\mapsto(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}\langle\theta^\varepsilon_z,\phi\rangle g^\varepsilon_z dz.$$

These operators are bounded operators on the functional spaces Σ^k_ε provided the family $(\theta^\varepsilon_z)_{\varepsilon>0}$ has nice properties.

Theorem 5.1. *Let $\varepsilon_0>0$.*

1. Compactly supported measurable families. *Let $R>0$. There exists $c_0>0$ such that for all measurable z-dependent family $(\theta^\varepsilon_z)_{\varepsilon>0}$, for all $k\in\mathbb{N}$, $\varepsilon\in(0,\varepsilon_0]$, for all $\phi\in L^2(\mathbb{R}^d)$*

$$\|\mathcal{J}[\theta^\varepsilon_z\mathbf{1}_{|z|<R}](\phi)\|_{\Sigma^k_\varepsilon}\leq(2\pi\varepsilon)^{-d}c_0\|\phi\|_{L^2}R^{2d}\sup_{|z|\leq R}\|\theta^\varepsilon_z\|_{\Sigma^k_\varepsilon}.$$

2. Wave packets. *Assume $\theta^\varepsilon_z=\lambda^\varepsilon(z)\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta)$ with $\theta\in\mathcal{S}(\mathbb{R}^d)$, $(\lambda^\varepsilon)_{\varepsilon>0}$ a bounded family in $L^\infty(\mathbb{R}^{2d},\mathbb{C})$ and Φ a smooth diffeomorphism of $\mathbb{R}^{2d}$ such that*

$$\exists c>0,\ \exists\ell\in\mathbb{N},\ \ \forall z\in\mathbb{R}^{2d},\ \ |J_\Phi(z)|+|J_\Phi(z)^{-1}|\leq c\langle z\rangle^\ell.$$

Then, there exists $c_0' > 0$ such that for all $\phi \in L^2(\mathbb{R}^d)$, $k \in \mathbb{N}$, $\varepsilon \in (0, \varepsilon_0]$,

$$\|\mathcal{J}[\theta_z^\varepsilon](\phi)\|_{\Sigma_\varepsilon^k} \le c_0' \,\|\lambda_\varepsilon\|_{L^\infty}\|\phi\|_{L^2}\|\theta\|_{\Sigma^{k+\ell+2d+1}}.$$

It turns out that for some families the set of integration in the Gaussian frame equality can be chosen compact. This is discussed in Appendix C.

Proof of Theorem 5.1. Let us first prove the L^2-estimate ($k = 0$) in both cases.
(1) By the Cauchy-Schwarz inequality, for $x \in \mathbb{R}^d$, we have

$$\begin{aligned}\|\mathcal{J}[\theta_z^\varepsilon \mathbf{1}_{|z|\le R}](\phi^\varepsilon)\|_{L^2}^2 &\le (2\pi\varepsilon)^{-2d}\|\phi\|_{L^2}^2 \int_{|z|,|z'|\le R}\left|\int_{x\in\mathbb{R}^d}\theta_z^\varepsilon(x)\overline{\theta_{z'}^\varepsilon}(x)dx\right| dz\,dz' \\ &\le (2\pi\varepsilon)^{-2d}\|\phi\|_{L^2}^2\int_{|z|,|z'|\le R}\|\theta_z^\varepsilon\|_{L^2}\|\theta_{z'}^\varepsilon\|_{L^2}\,dz\,dz' \\ &\le c_1 R^{4d}(2\pi\varepsilon)^{-2d}\|\phi\|_{L^2}^2\left(\sup_{|z|\le 2R}\|\theta_z^\varepsilon\|_{L^2}\right)^2\end{aligned}$$

where $c_1 > 0$ is a universal constant.
(2) Let $(x, y) \mapsto k^\varepsilon(x, y)$ be the integral kernel of the operator $\mathcal{J}[\theta_z^\varepsilon]$. Since the Bargmann transform is an isometry, it is equivalent to consider the operator

$$\mathcal{B}^\varepsilon \circ \mathcal{J}[\theta_z^\varepsilon] \circ \mathcal{B}_\varepsilon^*,$$

the kernel of which is the function $(\mathbb{R}^{2d})^2 \ni (X, Y) \mapsto k_{\mathcal{B}}^\varepsilon(X, Y)$ defined by

$$k_{\mathcal{B}}^\varepsilon(X,Y) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}\overline{g}_X^\varepsilon(x)g_Y^\varepsilon(y)k^\varepsilon(x,y)dxdy = (2\pi\varepsilon)^{-2d}\int_{z\in\mathbb{R}^{2d}}\langle g_z^\varepsilon, g_Y^\varepsilon\rangle\langle g_X^\varepsilon,\theta_z^\varepsilon\rangle dz.$$

Therefore, by (3.4), $k_{\mathcal{B}}^\varepsilon(X, Y)$ satisfies

$$|k_{\mathcal{B}}^\varepsilon(X,Y)| \le (2\pi\varepsilon)^{-2d}\int_{z\in\mathbb{R}^{2d}}\left|\lambda^\varepsilon(z)W[g_0,g_0]\left(\frac{Y-z}{\sqrt{\varepsilon}}\right)W[g_0,\theta]\left(\frac{\Phi(z)-X}{\sqrt{\varepsilon}}\right)\right|dz.$$

We deduce

$$\int_{\mathbb{R}^{2d}}|k_{\mathcal{B}}^\varepsilon(X,Y)|dX \le (2\pi)^{-2d}\|\lambda^\varepsilon\|_{L^\infty}\left(\int_{\mathbb{R}^{2d}}|W[g_0,g_0](z)|dz\right)\left(\int_{\mathbb{R}^{2d}}|W[g_0,\theta](X)|dX\right),$$

$$\int_{\mathbb{R}^{2d}}|k_{\mathcal{B}}^\varepsilon(X,Y)|dY \le M(2\pi)^{-2d}\|\lambda^\varepsilon\|_{L^\infty}\left(\int_{\mathbb{R}^{2d}}|W[g_0,g_0](Y)|dY\right)\left(\int_{\mathbb{R}^{2d}}|W[g_0,\theta](z)J_\Phi^{-1}(z)|dz\right),$$

and, by equations (3.5), we deduce the existence of $C > 0$ such that

$$\int_{\mathbb{R}^{2d}}|k_{\mathcal{B}}^\varepsilon(X,Y)|dX + \int_{\mathbb{R}^{2d}}|k_{\mathcal{B}}^\varepsilon(X,Y)|dY \le CM\|\theta\|_{\Sigma^{2d+\ell+1}}.$$

We then conclude by Schur Lemma and obtain

$$\|\mathcal{B}^\varepsilon \circ \mathcal{J}[\theta_z^\varepsilon]\circ(\mathcal{B}^\varepsilon)^*\|_{\mathcal{L}(L^2(\mathbb{R}^{2d}))} \le CM\ \|\lambda^\varepsilon\|_{L^\infty}\ \|\theta\|_{\Sigma^{2d+\ell+1}},$$

and so it is for $\mathcal{J}[\theta_z^\varepsilon]$.
(3) For concluding the proof when $k \ne 0$, we use that for $\alpha, \gamma \in \mathbb{N}^d$ and $\phi \in \mathcal{S}(\mathbb{R}^d)$,

$$x^\alpha(\varepsilon\partial_x)^\gamma\mathcal{J}[\theta_z^\varepsilon] = \mathcal{J}[x^\alpha(\varepsilon\partial_x)^\gamma\theta_z^\varepsilon],$$

with

$$x^\alpha(\varepsilon\partial_x)^\gamma\mathrm{WP}_z^\varepsilon(\theta) = \mathrm{WP}^\varepsilon\left((q+\sqrt{\varepsilon}x)^\alpha(p+\sqrt{\varepsilon}D_x)^\gamma\theta\right),$$

and one then concludes as in the proof of Lemma 3.1 by noticing that, if $|\alpha| + |\gamma| = k$, we have for all $n \in \mathbb{N}$,

$$\|(q+\sqrt{\varepsilon}x)^\alpha(p+\sqrt{\varepsilon}D_x)^\gamma\theta\|_{\Sigma^n} \le \langle z\rangle^k\|\theta\|_{\Sigma^{n+k}}.$$

This finishes the proof. □

These results extend to the adjoint of $\mathcal{J}[\theta_z^\varepsilon]$ (see (5.3) for its formula).

Corollary 5.2. *Under the assumptions of Theorem 5.1 (2), the family of operators* $\mathcal{J}[\theta_z^\varepsilon]^*$ *(see* (5.3)*) satisfies the same kind of estimates than the family* $\mathcal{J}[\theta_z^\varepsilon]$*.*

5.2. **Bargmann multipliers and classical flow.** In this section we analyze the properties of the operators $\mathcal{J}[\theta_z^\varepsilon]$ when $(\theta_z^\varepsilon)_{\varepsilon>0}$ is of the form

$$\theta_z^\varepsilon = \mathrm{e}^{\frac{i}{\varepsilon}S(z)}u(z)\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot)), \tag{5.4}$$

with $\theta \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathcal{S}(\mathbb{R}^d))$, $S \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{R})$, $u \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C})$ and Φ a smooth diffeomorphism satisfying the assumptions of Theorem 5.1. We are interested in the case where S and Φ are linked in the same manner as when they are the flow map and the action associated with classical trajectories. Therefore, we consider the following set of Assumptions.

(i) There exists $c > 0$ and $\ell \in \mathbb{N}$ such that

$$\forall z \in \mathbb{R}^{2d},\ \ |J_\Phi(z)| + |J_\Phi(z)^{-1}| \le c\langle z\rangle^\ell.$$

(ii) Setting $\Phi(z) = (\Phi_q(z), \Phi_p(z))$ and

$$\partial_z\Phi = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z)\end{pmatrix},$$

we have

$$\nabla_q S(z) = -p + A(z)\Phi_p(z) \ \text{ and } \ \nabla_p S(z) = B(z)\Phi_p(z),\ \ z = (q,p).$$

(iii) For all $k \in \mathbb{N}$, the quantities $\sup_{z\in\mathbb{R}^{2d}} \|\theta(z,\cdot)\|_{\Sigma^k}$, $\sup_{|\alpha|\le k} \|\partial_z^\alpha S\|_{L^\infty}$ and $\sup_{|\alpha|\le k} \|\partial_z^\alpha u\|_{L^\infty}$, are uniformly bounded in z.

We point out that the property (ii) is satisfied by the action associated with the flow map (see Section 4.5).

Lemma 5.3. *Let* $L = \partial_q - i\partial_p$*. Let* $\theta \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathcal{S}(\mathbb{R}^d))$*,* $S \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{R})$*,* $u \in \mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C})$ *and* Φ *a smooth diffeomorphism satisfying Assumptions (i), (ii) and (iii). Then, the following equality between operators in* $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_\varepsilon)$ *holds for* $k \in \mathbb{N}$*:*

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left((L\Phi_p x - L\Phi_q D_x)\theta\right)\right] = -i\sqrt{\varepsilon}\,\mathcal{J}\left[Lu\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(\theta)\right] - i\sqrt{\varepsilon}\,\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(L\theta)\right].$$

Note that we have

$$L\Phi_p(z) = C(z) - iD(z) \ \text{ and } \ L\Phi_q(z) = A(z) - iB(z). \tag{5.5}$$

Condition (ii) implies that the equality of Lemma 5.3 holds formally. Conditions (i) and (iii) ensure the boundedness of the operators involved in the estimates.

Proof. The integral kernel of the operator $\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(\theta)\right]$ is the function

$$(x,y) \mapsto \int_{z\in\mathbb{R}^{2d}} k(z,x,y)dz$$

defined by

$$k(z,x,y) = (2\pi\varepsilon)^{-d}u(z,x)\mathrm{e}^{\frac{i}{\varepsilon}S(z)}\overline{g_z^\varepsilon(y)}\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))(x),\ \ (x,y) \in \mathbb{R}^d,\ \ z \in \mathbb{R}^{2d}.$$

We aim at calculating Lk. We observe for $z=(q,p)\in\mathbb{R}^{2d}$, $y\in\mathbb{R}^d$ and

$$\begin{aligned} LS(z) &= -p+(A(z)-iB(z))L\Phi_p(z),\\ L\left(\overline{g_z^\varepsilon(y)}\right) &= \frac{i}{\varepsilon}[(Lp+iLq)(y-q)+pLq]g_z^\varepsilon(y)=\frac{i}{\varepsilon}p\,g_z^\varepsilon(y),\\ L\left(\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))\right) &= \mathrm{WP}^\varepsilon_{\Phi(z)}(L\theta(z,\cdot))+\frac{i}{\sqrt{\varepsilon}}\mathrm{WP}^\varepsilon_{\Phi(z)}\left((L\Phi_p(z)x-L\Phi_q(z)D_x)\theta(z,\cdot)\right)\\ &\quad -\frac{i}{\varepsilon}\mathrm{WP}^\varepsilon_{\Phi(z)}\left((A(z)-iB(z))L\Phi_p(z)\theta(z,\cdot)\right). \end{aligned}$$

We obtain

$$\begin{aligned} Lk(z,x,y) = \mathrm{e}^{\frac{i}{\varepsilon}S(z)}\Big(& Lu(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))(x)+u(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}(L\theta(z,\cdot))(x)\\ &+\frac{i}{\sqrt{\varepsilon}}u(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}\left((L\Phi_p(z)x-L\Phi_q(z)D_x)\theta(z,\cdot)\right)(x)\Big) \end{aligned}$$

The result then follows from the integration in $z\in\mathbb{R}^{2d}$. ☐

The case of Gaussian functions θ is of particular interest. Indeed, if $\theta(z,\cdot)=g^{\Theta(z)}$ with $\Theta\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathfrak{S}^+(d))$, we have for $x\in\mathbb{R}^d$ and $z\in\mathbb{R}^{2d}$,

$$(L\Phi_p(z)x-L\Phi_q(z)D_x)g^{\Theta(z)}(x)=(L\Phi_p(z)-L\Phi_q(z)\Theta(z))x\,g^{\Theta(z)}(x). \tag{5.6}$$

We set

$$M_\Theta(z):=L\Phi_p(z)-L\Phi_q(z)\Theta(z).$$

By (5.5), we have the equality between matrix-valued functions

$$M_\Theta=(C-iD)-(A-iB)\Theta=(A-iB)\left[(A-iB)^{-1}(C-iD)-\Theta\right]. \tag{5.7}$$

Note that this matrix M_Θ is invertible because $(A+iB)^{-1}(C+iD)-\overline{\Theta}\in\mathfrak{S}^+(d)$ (as the sum of two elements of $\mathfrak{S}^+(d)$). These observations are in the core of the proof of the next result which is a corollary of Lemma 5.3, when applied to Gaussian profiles.

Corollary 5.4. *Let $k\in\mathbb{N}$. Let $\Theta\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathfrak{S}^+(d))$ such that M_Θ is bounded together with its inverse, let $S\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{R})$, $u\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C})$ and Φ a smooth diffeomorphism satisfying Assumptions (i), (ii) and (iii). Then, in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_\varepsilon(\mathbb{R}^d))$, we have the following properties:*

(1) *For all $1\le j\le d$,*

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(x_j g^\Theta\right)\right]=\mathcal{O}(\sqrt{\varepsilon}). \tag{5.8}$$

(2) *For all $K\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C}^{d,d})$, in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_\varepsilon(\mathbb{R}^d))$, we have*

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(Kx\cdot xg^\Theta\right)\right]=\frac{1}{i}\,\mathcal{J}\left[u\,\mathrm{Tr}\left(K\,M_\Theta^{-1}\,L\Phi_q\right)\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(g^\Theta\right)\right]+\mathcal{O}(\varepsilon). \tag{5.9}$$

with

$$KM_\Theta^{-1}L\Phi_q=K\left[(A-iB)^{-1}(C-iD)-\Theta\right]^{-1}.$$

(3) *For all $\alpha\in\mathbb{N}^d$ with $|\alpha|=3$,*

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(x^\alpha g^\Theta\right)\right]=\mathcal{O}(\sqrt{\varepsilon}). \tag{5.10}$$

Remark 5.5. More can be said about the $\sqrt{\varepsilon}$-order term on the right-hand side of (5.8). By revisiting the proof below, one sees that there exists a real-valued smooth function $z\mapsto c(z)$ such that

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(xg^\Theta\right)\right]=-i\sqrt{\varepsilon}\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(c(z)g^\Theta\right)\right]+\mathcal{O}(\varepsilon).$$

Proof of Corollary 5.4. One uses (5.6) and Lemma 5.3 that we apply to $\theta = g^\Theta$. It gives that in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d))$, the following vector-valued relation holds

$$\mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left(xg^\Theta\right)\right] = \mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left(M_\Theta^{-1}(L\Phi_p x - L\Phi_q D_x)g^\Theta\right)\right] = \mathcal{O}(\sqrt{\varepsilon}),$$

whence (5.8).

Secondly, with $L \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{d,d})$, we associate the matrix K' such that $K = {}^tK' M_\Theta$. We have

$$\begin{aligned}(L\Phi_p x - L\Phi_q D_x)\cdot(K'xg^\Theta) &= \left(({}^tK'(L\Phi_p - L\Phi_q\Theta))x\cdot x - \mathrm{Tr}({}^tK' L\Phi_q)\right) g^\Theta\\ &= Kx\cdot x g^\Theta - \mathrm{Tr}(KM_\Theta^{-1}L\Phi_q)g^\Theta.\end{aligned}$$

It remains to prove that in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d))$, we have

$$\mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left((L\Phi_p x - L\Phi_q D_x)\cdot(K'xg^\Theta)\right)\right] = \mathcal{O}(\varepsilon). \tag{5.11}$$

We first apply Lemma 5.3 to the function $\theta = K'xg^\Theta$ and we write

$$\begin{aligned}&\mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left((L\Phi_p x - L\Phi_q D_x)\cdot(K'xg^\Theta)\right)\right]\\ &= -i\sqrt{\varepsilon}\mathcal{J}\left[Lu\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left(K'xg^\Theta\right) + u\mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left(K'x\, L(g^\Theta)\right)\right].\end{aligned}$$

We use the relation (5.8) and obtain in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d))$,

$$\mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left((L\Phi_p x - L\Phi_q D_x)\cdot(K'xg^\Theta)\right)\right] = -i\sqrt{\varepsilon}\mathcal{J}\left[u\mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left(K'x\, L(g^\Theta)\right)\right] + \mathcal{O}(\varepsilon). \tag{5.12}$$

We calculate

$$L(g^\Theta) = \frac{Lc_\Theta}{c_\Theta}g^\Theta + (L\Theta x\cdot x)g^\Theta,$$

with

$$\begin{aligned}(L\Theta x\cdot x)\, x\, g^\Theta &= (L\Theta x\cdot x)M_\Theta^{-1}(L\Phi_p x - L\Phi_q D_x)g^\Theta\\ &= M_\Theta^{-1}(L\Phi_p x - L\Phi_q D_x)\left((L\Theta x\cdot x)g^\Theta\right) - 2M_\Theta^{-1}L\Phi_q L\Theta\, x\, g^\Theta.\end{aligned}$$

Therefore, there exists matrices K_1 and K_2 such that, setting $\tilde\theta = (L\Theta x\cdot x)g^\Theta$, we have

$$K'x\, L(g^\Theta) = K_1 xg^\Theta + K_2(L\Phi_p x - L\Phi_q D_x)\tilde\theta.$$

We deduce

$$\mathcal{J}\left[u\, \mathrm{e}^{\frac{i}{\varepsilon}S}\, \mathrm{WP}^\varepsilon_\Phi\left((L\Phi_p x - L\Phi_q D_x)\cdot(K'xg^\Theta)\right)\right] = -i\sqrt{\varepsilon}\mathcal{J}[K_1xg^\Theta] - i\sqrt{\varepsilon}\mathcal{J}[K_2(L\Phi_p x - L\Phi_q D_x)\tilde\theta]$$

and we obtain (5.11) by Lemma 5.3 applied to the function $\tilde\theta$, and by the relation (5.8).

For treating a term with a coefficient x^β, with $|\beta| \geq 2$, we will use a recursive argument. Indeed, we have

$$(L\Phi_q x - L\Phi_p D_x)(x^\beta g^\Theta) = x^\beta(L\Phi_p - L\Phi_q\Theta)xg^\Theta - \sum_{|\beta'|=|\beta|-1} V_{\beta'}x^{\beta'}g^\Theta$$

for some vector-valued coefficient $V_{\beta'}$. We are left with the relation

$$(L\Phi_q x - L\Phi_p D_x)(x^\beta g^\Theta) = x^\beta M_\Theta xg^\Theta - \sum_{|\beta'|=|\beta|-1} V_{\beta'}x^{\beta'}g^\Theta. \tag{5.13}$$

We are interested in a term of the form $x^\alpha g^\Theta$ with $|\alpha| = 3$. We write $\alpha = \beta + e$, $|\beta| = 2$ and $|e| = 1$ and we consider the vector-valued function $x^\beta \, x g^\Theta$. We apply the relation (5.13) to $\beta \in \mathbb{N}^d$:

$$\begin{aligned} x^\beta \, x g^\Theta &= M_\Theta^{-1}(x^\beta \, M_\theta x g^\Theta) \\ &= M_\Theta^{-1}(L\Phi_q x - L\Phi_p D_x)(x^\beta g^\Theta) + \sum_{|\beta'|=1} M_\Theta^{-1} V_{\beta'} x^{\beta'} g^\Theta. \end{aligned}$$

Therefore, Lemma 5.3 and the first relation of the corollary gives the result. □

5.3. **Thawed Gaussian approximation.** We continue with the notation of Section 4.2 and keep the memory of the initial point of the classical trajectories. We consider the trajectories $z(t) = (q(t), p(t)) =: \Phi^t(z))$ when $z(0) = z$, the associated actions $S(t) =: S(t,z)$. We denote by $\Gamma(t,z)$ the width of the Gaussian profile associated with the initial data g_0 according to Remark 4.3. We define the operator

$$\mathcal{J}^t_{\rm th}(f) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} {\rm e}^{\frac{i}{\varepsilon} S(t,z)} \langle g^\varepsilon_z, f \rangle g^{\Gamma(t,z),\varepsilon}_{\Phi^t(z)} dz. \tag{5.14}$$

This operator belongs to the class of operators defined in Section 5.1 and we have

$$\mathcal{J}^t_{\rm th} = \mathcal{J}[\theta^\varepsilon_z(t)], \;\; \text{with} \;\; \theta^\varepsilon_z(t) = {\rm e}^{\frac{i}{\varepsilon} S(t,z)} g^{\Gamma(t,z),\varepsilon}_{\Phi^t(z)}.$$

In particular by Theorem 5.1 (2) and Lemmata 4.1 and 4.2, for all $t \in \mathbb{R}$, the operator $\mathcal{J}^t_{\rm th}$ is a bounded operator on the spaces Σ^k_ε.

It is proved in [22, 23] that the operator $\mathcal{J}^t_{\rm th}$ approximates the propagator ${\rm e}^{\frac{i}{t}\varepsilon \widehat{H}}$ where $\widehat{H}$ is the semiclassical Schrödinger operator $\widehat{H} = -\frac{\varepsilon^2}{2} + V(x)$ involved in equation (5.1).

Theorem 5.6. *For all $T \in \mathbb{R}$, there exists C_T such that the solution of* (5.1) *with initial data ψ^ε_0 satisfies*

$$\sup_{t \in [0,T]} \|\psi^\varepsilon(t) - \mathcal{J}^t_{\rm th}(\psi^\varepsilon_0)\|_{L^2(\mathbb{R}^d)} \leq C_T \|\psi^\varepsilon_0\|_{L^2} \varepsilon.$$

Proof. This result comes from combining elements described above. By the linearity of the integral, the frame identity (2.5) implies

$$\psi^\varepsilon(t,x) = {\rm e}^{-i\frac{t}{\varepsilon}\widehat{H}^\varepsilon} \psi^\varepsilon_0(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g^\varepsilon_z, \psi^\varepsilon_0 \rangle {\rm e}^{-i\frac{t}{\varepsilon}\widehat{H}^\varepsilon} g^\varepsilon_z(x) \, dz.$$

By Theorem 4.6, for all $z \in \mathbb{R}^{2d}$,

$${\rm e}^{-i\frac{t}{\varepsilon}\widehat{H}^\varepsilon} g^\varepsilon_z(x) = {\rm e}^{\frac{i}{\varepsilon}S(t,z)} g^{\varepsilon,\Gamma(t,z)}_{\Phi^t(z)} + {\rm e}^{\frac{i}{\varepsilon}S(t,z)} \sqrt{\varepsilon} \, {\rm WP}^\varepsilon_{\Phi^t(z)}(u_1(t,\cdot)) + \sqrt{\varepsilon} w^\varepsilon(t,\cdot))(x)$$

with $w^\varepsilon(t,\cdot) \in \mathcal{S}(\mathbb{R}^d)$ and for all $k \in \mathbb{N}$

$$\|w^\varepsilon(t,\cdot)\|_{\Sigma^k} \leq C_k \, \varepsilon.$$

Therefore, setting

$$\theta^\varepsilon_z(t,\cdot) = {\rm e}^{\frac{i}{\varepsilon}S(t,z)} \, {\rm WP}_{\Phi^t(z)}(u_1(t,\cdot)), \;\; z \in \mathbb{R}^{2d},,$$

we obtain by Theorem 5.1

$$\big\|\psi^\varepsilon(t,x) - \mathcal{J}^t_{\rm th}(\psi^\varepsilon_0) - \sqrt{\varepsilon} \, \mathcal{J}[\theta^\varepsilon_z(t,\cdot))]\psi^\varepsilon_0\big\|_{L^2(\mathbb{R}^d)} \leq C \, \varepsilon \, \|\psi^\varepsilon_0\|_{L^2(\mathbb{R}^d)}.$$

We conclude the proof by observing that Corollary 5.4 and Remark 4.7 imply that the operator $\mathcal{J}[\theta^\varepsilon_z(t,\cdot))]$ is of size $\sqrt{\varepsilon}$ in $\mathcal{L}(L^2(\mathbb{R}^d))$ for all $t \in \mathbb{R}$.

□

5.4. **Frozen Gaussian approximation.** The frozen Gaussian approximation is derived from the Thawed gaussian approximation by getting rid of the time-dependent variance matrices $\Gamma(t,z)$ at the proce of adding a scalar coefficient inn the integral. It was first proposed in [11], and then studied in [22, 23]. The so-called *Herman-Kluk prefactor* $a(t,z)$ is defined by

$$a(t,z) = 2^{-d/2}\mathrm{det}^{1/2}\left(A(t,z)+D(t,z)+i(C(t,z)-B(t,z)\right), \tag{5.15}$$

where $A(t,z)$, $B(t,z)$, $C(t,z)$ and $D(t,z)$ are the $d\times d$ matrices associated with the differential of the flow map according to (B.5). One then sets

$$\mathcal{J}^t_{\rm fr}(f) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\varepsilon}S(t,z)}\langle g^\varepsilon_z, f\rangle a(t,z) g^\varepsilon_{\Phi^t(z)} dz \tag{5.16}$$

Theorem 5.7. *For all $T\in\mathbb{R}$, there exists $C=C_T$ such that the solution of* (5.1) *with initial data ψ^ε_0 satisfies*

$$\sup_{t\in[0,T]}\|\psi^\varepsilon(t)-\mathcal{J}^t_{\rm fr}(\psi^\varepsilon_0)\|_{L^2(\mathbb{R}^d)}\leq C_T\|\psi^\varepsilon_0\|_{L^2}.$$

Proof. We use an argument of continuous perturbation for passing from $\mathcal{J}^t_{\rm th}$ to $\mathcal{J}^t_{\rm fr}$. We fix $t\in\mathbb{R}$ during all the proof. We set for $s\in[0,1]$

$$\Theta(s;t,z) = (1-s)\Gamma(t,z)+is\mathrm{Id},$$

so that $\Theta(0,z)=\Gamma(t,z)$, as the width of the Gaussian involved in $\mathcal{J}^t_{\rm th}$, and $\Theta(1,s)=i\mathrm{Id}$, as the width of the Gaussian in $\mathcal{J}^t_{\rm fr}$. We consider the partially normalised Gaussian function

$$\widetilde{g}(s;t,y) = (\pi)^{-d/4}\mathrm{e}^{\frac{i}{2}\Theta(s,z)y\cdot y},\ y\in\mathbb{R}^d.$$

The aim is to construct a map $s\mapsto b(s;t,z)$ such that for all $s\in[0,1]$ in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\frac{d}{ds}\mathcal{J}\left[\theta^\varepsilon_z(s;t)\right] = \mathcal{O}(\varepsilon)\ \text{ with }\ \theta^\varepsilon_z(s;t,\cdot) = b(s;t,z)\mathrm{WP}^\varepsilon_{\Phi^t(z)}\left(\widetilde{g}(s;t,\cdot)\right),$$

Choosing $b(0;t,z)=1$, we have

$$\mathcal{J}^t_{\rm th} = \mathcal{J}\left[\theta^\varepsilon_z(0;t,\cdot)\right],$$

and we will obtain in $\mathcal{L}(L^2(\mathbb{R}^d))$ for all $s\in[0,1]$,

$$\mathcal{J}^t_{\rm th} = \mathcal{J}\left[\theta^\varepsilon_z(s;t,\cdot)\right]+\mathcal{O}(\varepsilon) = \mathcal{J}^t_{\rm fr}+\mathcal{O}(\varepsilon)$$

provided $b(1;t,z)$ coincides with the Herman-Kluk prefactor $a(t,z)$ defined in (5.15). For constructing the map $s\mapsto b(s;t,z)$, we compute

$$\frac{d}{ds}\mathcal{J}\left[\theta^\varepsilon_z(s;t,\cdot)\right] = \mathcal{J}\left[\partial_z\theta^\varepsilon_z(s;t,\cdot)\right]$$

with

$$\partial_z\theta^\varepsilon_z(s;t,\cdot) = \partial_s b(s;t,z)\mathrm{WP}^\varepsilon_{\Phi^t(z)}\left(\widetilde{g}(s;t,y)\right)++\frac{i}{2}b(s;t,z)\mathrm{WP}^\varepsilon_{\Phi^t(z)}\left(\partial_s\Theta(s;t,z)y\cdot y\widetilde{g}^{\Theta(s)}(s;t,y)\right).$$

We use equation (5.9) of Corollary 5.4 to transform the second term of the right-hand side and obtain

$$\mathcal{J}\left[b(s;t,z)\mathrm{WP}^\varepsilon_{\Phi^t(z)}(\partial_s\Theta(s;t,z)y\cdot y\,\widetilde{g}(s;t,y))\right] = \frac{1}{i}\mathcal{J}\left[b(s;t,z)\mathrm{WP}^\varepsilon_{\Phi^t(z)}(\mathrm{Tr}(\Theta_1(s))\widetilde{g}(s;t,y))\right]+\mathcal{O}(\varepsilon)$$

in $\mathcal{L}(L^2(\mathbb{R}^d))$ and with

$$\Theta_1(s;t,z) = \partial_s\Theta(s;t,z)\left[(A(t,z)-iB(t,z))^{-1}(C(t,z)-iD(t,z))-\Theta(s;t,z)\right]^{-1}.$$

Let $M(s;t,z)$ be the matrix associated with $\Theta(s;t,z)$ according to (5.7). We have

$$\partial_s M(s;t,z) = -(A(t,z)-iB(t,z))\partial_s\Theta(s;t,z).$$

We deduce

$$\Theta_1(s;t,z) = -(A(t,z) - iB(t,z))^{-1}\partial_s M(s;t,z)M(s;t,z)^{-1}(A(t,z) - iB(t,z))$$

and

$$\mathrm{Tr}(\Theta_1(s;t,z)) = -\mathrm{Tr}(\partial_s M(s;t,z)M(s;t,z)^{-1}) = -\mathrm{det}M(s;t,z)^{-1}\,\partial_s\left(\mathrm{det}M(s;t,z)\right).$$

Therefore, the condition

$$\partial_s b(s;t,z) - \frac{1}{2}\mathrm{Tr}(\partial_s M(s;t,z)M(s;t,z)^{-1})b(s;t,z) = 0$$

that we have to fulfilled, is realized by

$$b(s;t,z) = \frac{\mathrm{det}M(s;t,z)}{\mathrm{det}M(0;t,z)}b(0;t,z), \quad s \in [0,1],$$

and we have $b(1;t,z) = a(t,z)$, as expected. □

APPENDIX A. DEVOIR

On considère l'ensemble $\mathcal{A}$ des fonctions $a \in \mathcal{C}^\infty(\mathbb{R}^{3d})$ vérifiant les deux propriétés :

(i) Il existe un compact $K \subset \mathbb{R}^{2d}$ tel que pour tout $\eta \in \mathbb{R}^d$, $(x,\xi) \mapsto a(x,\xi,\eta)$ est à support dans K.

(ii) Il existe $R_0 > 0$ tel que si $|\eta| > R_0$, alors

$$\forall (x,\xi) \in K, \ \ a(x,\xi,\eta) = a\left(x,\xi,\frac{\eta}{|\eta|}\right).$$

On utilise dans cet exercice la quantification de Weyl.

A. On note $a_\varepsilon(x,\xi) = a\left(x,\xi,\frac{x}{\sqrt{\varepsilon}}\right)$ et on considère l'opérateur T^ε défini sur $L^2(\mathbb{R}^d)$ par

$$T^\varepsilon f(x) = \varepsilon^{d/4} f(\sqrt{\varepsilon}x), \ \ \forall f \in L^2(\mathbb{R}^d), \ \ \forall x \in \mathbb{R}^d.$$

(1) Montrer que le noyau de l'opérateur $T^\varepsilon \mathrm{op}_\varepsilon(a_\varepsilon)(T^\varepsilon)^*$ est de la forme

$$(x,y) \mapsto \varepsilon^{-d/2} k_\varepsilon\left(\frac{x+y}{2}, \frac{x-y}{\sqrt{\varepsilon}}\right)$$

pour une fonction $k_\varepsilon \in \mathcal{S}(\mathbb{R}^{2d})$ que l'on calculera en fonction de ε.

(2) Montrer que $(X,v) \mapsto k_\varepsilon(X,v)$ est bornée uniformément en ε sur le compact $\{|v| \le 1\}$.

(3) Soit $N \in \mathbb{N}$, montrer que $(X,v) \mapsto |v|^{2N} k_\varepsilon(X,v)$ est bornée uniformément en ε sur l'ensemble $\{|v| \ge 1\}$.

(4) Déduire des questions précédentes:

$$\exists C > 0, \ \ \forall \varepsilon > 0, \ \ \int_{\mathbb{R}^d} \sup_{X \in \mathbb{R}^d} |k_\varepsilon(X,v)| dv \le C.$$

(5) Montrer que la famille d'opérateurs $T^\varepsilon \mathrm{op}_\varepsilon(a_\varepsilon)(T^\varepsilon)^*$ est bornée dans $\mathcal{L}(L^2(\mathbb{R}^d))$ et en déduire qu'il en est de même pour $(\mathrm{op}_\varepsilon(a_\varepsilon))_{\varepsilon>0}$.

A bis (préparatoire au B). Soit $a \in \mathcal{A}$.

(1) Montrer qu'il existe une fonction $b_\varepsilon \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ telle que

$$T^\varepsilon \mathrm{op}_\varepsilon(a_\varepsilon)(T^\varepsilon)^* = \mathrm{op}_{\sqrt{\varepsilon}}(b_\varepsilon).$$

(2) On note $\mathrm{op}^{\mathrm{KN}}$ la quantification de Kohn-Niremberg (ou quantification classique). Montrer que

$$\mathrm{op}_\varepsilon(a_\varepsilon) = \mathrm{op}_\varepsilon^{\mathrm{KN}}(a_\varepsilon) + O(\sqrt{\varepsilon})$$

dans $L^2(\mathbb{R}^d)$. On pourra utiliser les résultats du cours pour le paramètre semi-classique $\sqrt{\varepsilon}$.

B. Soit $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $(x_0,\xi_0,\omega_0) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$ et $\beta \in (0,1]$. On pose

$$u^\varepsilon(x) = \varepsilon^{-d/4} \varphi\left(\frac{x - x_0 - \varepsilon^\beta \omega_0}{\sqrt{\varepsilon}}\right) \exp\left(i\frac{x\cdot\xi_0}{\varepsilon}\right), \ \ \forall x \in \mathbb{R}^d.$$

(1) Montrer que $(u^\varepsilon)_{\varepsilon>0}$ est une famille bornée de $L^2(\mathbb{R}^d)$.

(2) Soit $b \in \mathcal{S}(\mathbb{R}^{2d})$, déterminer la limite de $(\mathrm{op}_\varepsilon(b)u^\varepsilon, u^\varepsilon)$ suivant les valeurs de β.

(3) Soit $a \in \mathcal{A}$. On choisit $x_0 = 0$, $\omega_0 \neq 0$. Déterminer suivant les valeurs de β la limite de $(\mathrm{op}_\varepsilon(a_\varepsilon)u^\varepsilon, u^\varepsilon)$ lorsque ε tend vers 0.

Exercice 1 - Retour sur la propagation des paquets d'onde.

(1) Montrer que si $\psi^\varepsilon = \mathrm{WP}_z(\varphi)$ pour un certain $z=(q,p)\in\mathbb{R}^{2d}$ et une fonction $\varphi\in\mathcal{S}(\mathbb{R}^d)$, alors
$$\forall y\in\mathbb{R}^d, \varphi(y) = \varepsilon^{\frac{d}{4}}\mathrm{e}^{-\frac{i}{\sqrt{\varepsilon}}p\cdot y}\psi^\varepsilon(q+\sqrt{\varepsilon}y).$$

(2) En utilisant la question précédente, montrer que si $a\in\mathcal{S}(\mathbb{R}^{2d})$, $z=(q,p)\in\mathbb{R}^{2d}$ et $\varphi\in\mathcal{S}(\mathbb{R}^d)$,
$$\mathrm{op}_\varepsilon^{\mathrm{w}}(a)\mathrm{WP}_z(\varphi) = \mathrm{WP}_z(\mathrm{op}_1^{\mathrm{w}}(a_{\varepsilon,z})\varphi)$$
avec $a_{\varepsilon,z}(y,\eta) = a(q+\sqrt{\varepsilon}y, p+\sqrt{\varepsilon}\eta)$. Vérifier que les semi-normes de Schwartz de la fonction $\mathrm{op}_1^{\mathrm{w}}(a_{\varepsilon,z})\varphi$ sont uniformément bornées par-rapport à ε.

(3) Soit u une fonction de $L^2(\mathbb{R}^d)$ telle que
$$i\partial_t u(t,y) = -\frac{1}{2}\Delta u(t,y) + B(t)y\cdot y\, u(t,y) + L(t,y)u(t,y) + f(t,y),\ \ u(0,y)=u_0.$$
où $t\mapsto B(t)$ et $(t,y)\mapsto L(t,y)$ sont continues et bornées, et $t\mapsto f(t,\cdot)$ continue de $\mathbb{R}$ dans $\Sigma^1(\mathbb{R}^d)$. On suppose que $u(0,\cdot)\in\Sigma^1(\mathbb{R}^d)$. Montrer que pour tout $t\in\mathbb{R}$, $u(t,\cdot)\in\Sigma^1(\mathbb{R}^d)$ et donner une estimation de $\|u(t,\cdot)\|_{\Sigma^1}$.

(4) Vérifier la récurrence de la dernière preuve du cours de la semaine dernière (Théorème 4.6).

Exercice 2 - Solutions gaussiennes de l'équation de profil. On considère l'équation de profil associée à l'équation de Schrödinger du cours précédent avec une donnée initiale gaussienne
$$i\partial_t u(t,y) = -\frac{1}{2}\Delta u(t,y) + \frac{1}{2}V''(q(t))y\cdot y\, u(t,y),\ \ u(0,y) = c_0\mathrm{e}^{\frac{i}{2}\Gamma_0 y\cdot y} \tag{B.1}$$
où Γ_0 est dans l'espace de Siegel des matrices symétriques de $\mathbb{C}^{d,d}$ à partie imaginaire strictement positive, et $c_0\in\mathbb{C}$ choisi pour que $\|u(0,\cdot)\|_{L^2}=1$.

(1) Montrer que si $u(t,y) = c(t)\mathrm{e}^{\frac{i}{2}\Gamma(t)y\cdot y}$ est solution de l'équation avec $\Gamma(t)$ une matrice complexe symétrique, alors les applications $t\mapsto\Gamma(t)$ et $t\mapsto c(t)$ vérifient
$$\begin{aligned}&\dot\Gamma(t) + \Gamma(t)^2 + V''(q(t)) = 0,\ \ \Gamma(0)=\Gamma_0,\\ &\dot c(t) = -\frac{1}{2}c(t)\,\mathrm{Tr}\,\Gamma(t),\ \ c(0)=c_0.\end{aligned} \tag{B.2}$$

La suite de l'exercice vise à résoudre l'équation (B.2) dans l'espace de Siegel.

(2) **Caractérisation de l'espace de Siegel**. Soit Q et P deux matrices de $\mathbb{C}^{d,d}$ telle que la matrice de $\mathbb{R}^{2d,2d}$
$$Y = \begin{pmatrix}\mathrm{Re}\,Q & \mathrm{Im}\,Q\\ \mathrm{Re}\,P & \mathrm{Im}\,P\end{pmatrix} \tag{B.3}$$
soit symplectique. Montrer qu'alors Q et P sont inversibles et $C=PQ^{-1}$ est dans l'espace de Siegel avec
$$\mathrm{Im} C = (QQ^*)^{-1}. \tag{B.4}$$
Réciproquement, montrer que toute matrice complexe symétrique C à partie imaginaire définie positive s'écrit $C=PQ^{-1}$ avec Q et P vérifiant (B.3) et (B.4).

On vérifiera que la condition (B.3) équivaut à

$$ {}^tQP - {}^tPQ = 0 \text{ et } Q^*P - P^*Q = 2i\,\mathrm{Id}, $$

et on remarquera que la factorisation (B.4) n'est pas unique car on peut multiplier Q et P par une matrice unitaire tout en conservant (B.3).

(3) Supposons que la donnée initiale de l'équation (B.2) s'écrive $\Gamma_0 = P_0Q_0^{-1}$ d'après la question précédente. Montrer que $\Gamma(t) = P(t)Q(t)^{-1}$ avec

$$ \dot{Q}(t) = P(t),\ \ \dot{P}(t) = -V''(q(t))Q(t),\ \ Q(0) = Q_0\ \ P(0) = P_0, $$

fournit une solution de l'équation (B.4) qui est bien dans l'espace de Siegel. Vérifier que l'on peut prendre $c(t) = \pi^{-d/4}(\det Q(t))^{-1/2}$.

(4) Vérifier qu'en prenant comme donnée initiale la matrice $\Gamma(0) = i\mathrm{Id}$, la solution précédente coincide avec la fonction $\Gamma(t)$ construite comme suit: soit $F(t, z)$ satisfaisant au système

$$ \partial_t F(t,z) = \begin{pmatrix} 0 & \mathrm{Id}_{\mathbb{R}^d} \\ -\mathrm{Hess}V(q(t)) & 0 \end{pmatrix} F(t,z),\ \ F(0,z) = \mathrm{Id}_{\mathbb{R}^{2d}}, $$

posons

$$ F(t,z) = \begin{pmatrix} A(t,z) & B(t,z) \\ C(t,z) & D(t,z) \end{pmatrix} \tag{B.5} $$

alors

$$ \begin{aligned} \Gamma(t) &= (C(t,z) + iD(t,z))(A(t,z) + iB(t,z))^{-1}, \\ c(t) &= \pi^{-\frac{d}{4}}\det{}^{-1/2}(A(t,z) + iB(t,z). \end{aligned} $$

On remarquera que la fonction $F(t, z) = \partial_z\Phi^t(z) \in \mathbb{R}^{2d}$ où $\Phi^t(z) = (q(t), \dot{p}(t))$, $\dot{q}(t) = p(t)$ et $\dot{p}(t) = -\nabla V(q(t))$ vérifie bien le système considéré. La matrice $\Gamma(t)$ peut donc se calculer à partir des équations des trajectoires classiques, en les dérivant.

Exercice 3 - Paquets d'onde de Hagedorn. On va construire une base Hilbertienne de solutions de l'équation (B.1). Si Q et P sont des matrices satisfaisant à (B.3) et (B.4), $q, p \in \mathbb{R}^d$, on introduit l'*échelle de Hagedorn*, c'est à dire l'ensemble de ces $2d$ opérateurs

$$ \mathcal{A} = -\frac{i}{\sqrt{2}}({}^tP(y-q) - {}^tQ(D_y - p)),\ \ \mathcal{A}^* = \frac{i}{\sqrt{2}}(P^*(y-q) - Q^*(D_y - p)). $$

On notera $\mathcal{A} = (\mathcal{A}_1, \cdots, \mathcal{A}_d)$ et $\mathcal{A}^* = (\mathcal{A}_1^*, \cdots, \mathcal{A}_d^*)$. Dans la suite, on suppose $q = p = 0$.

(1) **Préliminaires**. Vérifier que si $d = 1$, $Q = 1$, $P = i$, $\mathcal{A}$ et $\mathcal{A}^*$ sont les opérateurs de création et d'annihillation associés à l'oscillateur harmonique $x^2 - \partial_x^2$. Vérifier que $\mathcal{A}_j^*$ est bien l'adjoint de $\mathcal{A}_j$, et que $[\mathcal{A}_j, \mathcal{A}_k^*] = \delta_{jk}$.

(2) On pose $\Gamma = PQ^{-1}$, et, pour $y \in \mathbb{R}^d$, $\varphi_0[Q, P](y) = ce^{\frac{i}{2}\Gamma y\cdot y}$ où c est choisi pour que $\|\varphi_0\|_{L^2} = 1$. Montrer les relations suivantes

$$ \mathcal{A}e^{\frac{i}{2}\Gamma y\cdot y} = 0,\ \ \mathcal{A}_j\mathcal{A}_j^*\varphi_0 = \varphi_0,\ \ \mathcal{A}_j\mathcal{A}_\ell^*\varphi_0 = \mathcal{A}_j^*\mathcal{A}_\ell\varphi_0 = 0,\ \ 1 \le j \ne \ell \le d. $$

(3) **Fonctions de Hagedorn**. On note e_j le multi-index $e_j = (0, \cdots, 1, \cdots, 0)$ avec un 1 à la j-ième place, et on construit la famille $(\varphi_k)_{k\in\mathbb{N}^d}$ par récurrence en partant de φ_0 et en posant

$$ \varphi_{k+e_j} = \frac{1}{\sqrt{k_j + 1}}\mathcal{A}_j^*\varphi_k,\ \ k \in \mathbb{N}^d,\ \ 1 \le j \le d. $$

Montrer que φ_{e_j} est dans le noyau de $\mathcal{A}_\ell^*\mathcal{A}_\ell$ si $\ell \neq j$, et est vecteur propre de $\mathcal{A}_j^*\mathcal{A}_j$ pour la valeur propre 1. Vérifier les relations (lorsqu'elles ont un sens)

$$\mathcal{A}_j\mathcal{A}_j^*\varphi_k = (k_j+1)\varphi_k, \;\; \mathcal{A}_j^*\mathcal{A}_j\varphi_k = k_j\varphi_k, \;\; \varphi_{k-e_j} = \frac{1}{\sqrt{k_j}}\mathcal{A}_j\varphi_k, \;\; k \in \mathbb{N}^d, \;\; 1 \leq j \leq d.$$

Montrer que la famille $(\varphi_k)_{k\in\mathbb{N}^d}$ est orthonormée.

(4) Montrer qu'il existe une famille de polynômes φ_k de degrés $|k| = k_1 + \cdots + k_d$ tels que

$$\varphi_k(y) = \frac{1}{\sqrt{2^{|k|}k!}}p_k(Q^{-1}y)\varphi_0(y), \;\; y \in \mathbb{R}^d.$$

Montrer que la famille $(\varphi_k)_{k\in\mathbb{N}^d}$ est une base Hilbertienne.

(5) Que se passe-t-il si q et p ne sont pas nuls?

Exercice 4 - Existence de solutions pour l'équation de Schrödinger avec potentiel quadratique dépendant du temps. On veut résoudre l'équation (B.1) avec une donnée L^2 quelconque. On considère la solution gaussienne construite à l'Exercice 2, que l'on note $\varphi_0(t,y)$, ainsi que les matrices $Q(t)$ et $P(t)$ associées. On choisit la base $(\varphi_k(t,\cdot))_{k\in\mathbb{N}^d}$ construite à l'aide des matrices $Q(t)$, $P(t)$ dans l'Exercice 3, et en prenant $q = p = 0$. Montrer que pour tout $1 \leq j \leq d$,

$$\dot{\mathcal{A}}_j(t) = \frac{1}{i}[\mathcal{A}_j, H] \;\text{ et }\; \dot{\mathcal{A}}_j^* = -\frac{1}{i}[\mathcal{A}_j^*, H].$$

Montrer que les fonctions $\varphi_k(t,\cdot)$ donnent une base hilbertienne de solutions de l'équation (B.1) En déduire l'existence d'une solution pour toute donnée initiale dans $L^2(\mathbb{R})$. Que peut-on dire si $u_0 \in \mathcal{S}(\mathbb{R}^d)$?

Remarque. En ajoutant au bon endroit le paramètre semi-classique, en faisant varier les points $q(t$ et $p(t)$ et en ajoutant l'action classique, on peut construire ainsi des base Hilbertiennes de solutions approchées d'une équation de Schrödinger semi-classique à potentiel sous-quadratique. Pour lus de détails, on renvoie à l'article de review de Caroline Lasser et Christian Lubich, *Computing quantum dynamics in the semiclassical regime*, Acta Numerica, 2020.

Examen

30 mars 2026 – 3 heures – documents autorisés
On pourra admettre le résultat d'une question et continuer l'exercice.

Le but de ce problème est d'analyser un système de deux équations aux dérivées partielles couplées.

A) On travaille dans $L^2(\mathbb{R})$. Déterminer s'il existe un état cohérent solution de l'équation

$$i\varepsilon\partial_t\psi^\varepsilon(t,x)) = (\varepsilon D_x + x)\psi^\varepsilon(t,x), \;\; \psi_1^\varepsilon(0,\cdot) = \mathrm{WP}_{z_0}(\varphi), \;\; x \in \mathbb{R},$$

où $\varphi \in \mathcal{S}(\mathbb{R})$ et $z_0 = (q_0, p_0) \in \mathbb{R}^2$. On notera $z(t)$, $\varphi(t,\cdot)$ les paramètres du paquet d'onde et $S(t)$ l'action.

B) On travaille maintenant dans $L^2(\mathbb{R}, \mathbb{C}^2)$. On dit que $f = {}^t(f_1, f_2) \in L^2(\mathbb{R}, \mathbb{C}^2)$ si $f_1 \in L^2(\mathbb{R})$ et $f_2 \in L^2(\mathbb{R})$, et, en notant $|\cdot|_{\mathbb{C}^2}$ la norme hermitienne sur $\mathbb{C}^2$, on pose

$$\|f\|^2_{L^2(\mathbb{R},\mathbb{C}^2)} = \|f_1\|^2_{L^2(\mathbb{R})} + \|f_2\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} |f(t,x)|^2_{\mathbb{C}^2} dx.$$

Dans $L^2(\mathbb{R}, \mathbb{C}^2)$, pour $z \in \mathbb{R}^2$, $\varphi \in \mathcal{S}(\mathbb{R})$ et $\vec{V} = {}^t(V_1, V_2) \in \mathcal{C}^\infty(\mathbb{R}, \mathbb{C}^2)$, on notera $\mathrm{WP}_z(\varphi\vec{V})$ la fonction à valeurs dans $\mathbb{C}^2$ dont les composantes sont $\mathrm{WP}_z(\varphi V_1)$ et $\mathrm{WP}_z(\varphi V_2)$.
Dans cette partie, Ω est une fonction C^∞ bornée, de $\mathbb{R}$ dans l'ensemble des matrices symétriques réelles, et dont les dérivées à tout ordre sont bornées,

(1) Montrer que si $z = (q,p) \in \mathbb{R}^2$, $\varphi \in \mathcal{S}(\mathbb{R})$ et $\vec{V} \in \mathbb{C}^2$, on a les propriétés suivantes

$$\begin{aligned}
&(a) \;\; \Omega(x)\mathrm{WP}_z(\varphi)(x)\vec{V} = \Omega(x)\mathrm{WP}_z(\varphi\vec{V})(x), \;\; \forall x \in \mathbb{R},\\
&(b) \;\; \|\Omega\mathrm{WP}_z(\varphi)\vec{V}\|_{L^2(\mathbb{R},\mathbb{C}^2)} \le \sup_{x\in\mathbb{R}} |\Omega(x)|_{\mathbb{C}^{2,2}} \|\vec{V}\|_{\mathbb{C}^2} \|\varphi\|_{L^2},\\
&(c) \;\; \Omega(x)\,\mathrm{WP}_z(\varphi)(x)\vec{V} = \mathrm{WP}_z(\varphi)(x)\Omega(q)\vec{V} + \sqrt{\varepsilon}\, r^\varepsilon(x), \;\; \forall x \in \mathbb{R},\\
&\quad\;\;\; \text{avec } \; \|r^\varepsilon\|_{L^2(\mathbb{R},\mathbb{C}^2)} = O(1),
\end{aligned}$$

où l'on a noté $|M|_{\mathbb{C}^{2,2}} = \sup_{1\le i,j\le 2} |M_{i,j}|$ la norme matricielle.
Dans (c) peut-on pousser le développement à l'ordre ε ? Si oui, écrire le terme d'ordre $\sqrt{\varepsilon}$.

(2) Soit $s \in \mathbb{R}$. On considère l'équation différentielle sur l'ensemble des matrices 2×2

$$i\partial_t U(t,s) = \Omega(t)U(t,s), \;\; U(s,s) = \mathrm{Id}_{\mathbb{C}^2}.$$

Montrer qu'il existe $\tau > 0$ tel que pour tout $s \in \mathbb{R}$ cette équation a une solution sur l'intervalle $[s, s+\tau]$. Montrer que pour tout $s \in \mathbb{R}$ et $t \in [s, s+\tau]$, $U(t,s)$ est unitaire. En déduire que l'on peut prendre $\tau = +\infty$.

C) On considère le système d'équations dans $L^2(\mathbb{R}, \mathbb{C}^2)$ donné par

$$\begin{aligned}
(E) \qquad & i\varepsilon\partial_t\psi^\varepsilon(t,x) = \left((\varepsilon D_x + x)\mathrm{Id}_{\mathbb{C}^2} + \varepsilon\Omega(x)\right)\psi^\varepsilon(t,x), \;\; (t,x) \in \mathbb{R}\times\mathbb{R},\\
& \psi^\varepsilon(0,\cdot) = \mathrm{WP}_{z_0}(\varphi)\vec{e}, \;\; \varphi \in \mathcal{S}(\mathbb{R}), \;\; z_0 = (0,0), \;\; \vec{e} \in \mathbb{C}^2.
\end{aligned}$$

(1) Vérifier que sous condition d'existence, on a bien $\|\psi^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R},\mathbb{C}^2)} = \|\psi^\varepsilon(0,\cdot)\|_{L^2(\mathbb{R},\mathbb{C}^2)}$ et exprimer cette norme en fonction de φ et $\vec{e}$.

(2) Montrer que

$$\forall T > 0, \;\; \exists C_T > 0, \;\; \sup_{t\in[0,T]} \|\psi^\varepsilon(t,\cdot) - \mathrm{e}^{\frac{i}{\varepsilon}S(t)}\mathrm{WP}_{z(t)}(\varphi(t,\cdot))\vec{e}(t)\,\|_{L^2(\mathbb{R},\mathbb{C}^2)} \le C_T\sqrt{\varepsilon},$$

où $\varphi(t,\cdot) \in \mathcal{S}(\mathbb{R})$, $S(t) \in \mathbb{R}$, $z(t) \in \mathbb{R}^2$ sont les paramètres de la question A pour un certain z_0 que l'on précisera, et $\vec{e}(t) = U(t,0)\vec{e}$ ($U(t,s)$ est la matrice unitaire introduite à la partie B).

(3) On cherche à améliorer cette approximation. Trouver des conditions que doivent vérifier $u(t,\cdot)$ et $\vec{V}(t,\cdot)$ pour que la fonction

$$(i) \qquad \psi^{\varepsilon}_{1,\mathrm{app}} = \mathrm{e}^{\frac{i}{\varepsilon}S(t)} \Big(\mathrm{WP}_{z(t)}(\varphi(t,\cdot))U(t)\vec{e} + \sqrt{\varepsilon}\,\mathrm{WP}_{z(t)}(u(t,\cdot))\vec{V}(t)\Big)$$

approche $\psi^{\varepsilon}(t,\cdot)$ à $O(\varepsilon)$ près (on établira une ODE pour $\vec{V}(t)$, on les résoudra en utilisant l'application $(t,s) \mapsto U(t,s)$ et la formule de Duhamel).

(4) Que devient ce résultat si l'on prend $z_0 = (q,p)$ quelconque pour la donnée initiale de l'équation (E) ?

D) On veut maintenant construire un opérateur intégral de Fourier approchant les solutions de l'équation (E) pour des données $\psi \in L^2(\mathbb{R},\mathbb{C}^2)$ quelconques.

(1) Expliquez pourquoi il est suffisant de traiter le cas $\psi(x) = f(x)\vec{e}$ où $\vec{e}$ est n'importe quel vecteur fixé de $\mathbb{C}^2$ et $f \in L^2(\mathbb{R})$ quelconque.

(2) En utilisant la famille des gaussiennes $(g^{\varepsilon}_{z})_{\varepsilon>0,\, z\in\mathbb{R}^2}$ proposer une représentation intégrale des solutions de (E) avec donnée $f(x)\vec{e}$ à $O(\varepsilon)$ près dans $L^2(\mathbb{R},\mathbb{C}^2)$.

Appendix C. Frequency localized families

The estimate (1) of Theorem 5.1 suggests to consider families of initial data for which the frame identity (2.5) can be taken compactly supported with a reasonable (controlled) error. This is realized by the notion of frequency localized families.

Definition C.1. Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$. We say that $(\phi^\varepsilon)_{\varepsilon>0}$ is *frequency localized at the scale* $\beta \geq 0$ if there exists constants $R_\beta, C_\beta, \varepsilon_\beta > 0$, $N_\beta \in \mathbb{N}$, $N_\beta > d + \frac{1}{2}$ such that for $|z| > R_\beta$ and $\varepsilon \in (0, \varepsilon_\beta]$,

$$|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)| \leq C_\beta\, \varepsilon^\beta \, \langle z \rangle^{-N_\beta}.$$

In other words, if $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$, its Bargmann transform has polynomial decay at infinity and is controlled by ε^β outside a ball $B(0, R_\beta)$.

The set of frequency localized functions is a subspace of $L^2(\mathbb{R}^d)$. Moreover, in view of

$$\left|\langle g^\varepsilon_{q,p}, \phi^\varepsilon \rangle\right| = \left|\langle g^\varepsilon_{p,-q}, \mathcal{F}^\varepsilon \phi^\varepsilon \rangle\right|$$

it is stable under the action of the ε-Fourier transform. Moreover, one has the two following properties:

1. If $(\phi_1^\varepsilon)_{\varepsilon>0}$ and $(\phi_2^\varepsilon)_{\varepsilon>0}$ are two frequency localized families at the scales β_1 and β_2 respectively, then for all $a, b \in \mathbb{C}$, the family $(a\phi_1^\varepsilon + b\phi_2^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\min(\beta_1, \beta_2)$.
2. If $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$, then it is also frequency localized at the scale β' for all $\beta' \in [0, \beta]$.

The relation of this notion with respect to the decomposition on the Gaussian frame stated as follows.

Lemma C.2. *Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a frequency localized family at the scale $\beta \geq 0$. Let R_β, C_β and N_β be the constants associated to $(\phi^\varepsilon)_{\varepsilon>0}$ according to Definition C.1. Let $k \in \mathbb{N}$ with $N_\beta > d + k$. Then, for all $\chi \in L^\infty(\mathbb{R})$ supported in $[0, 2]$ and equal to 1 on $[0, 1]$, there exists $C > 0$ such that for $R > R_\beta$ and $\varepsilon \in (0, 1]$,*

$$\left\| \phi^\varepsilon - \mathcal{J}\left[g^\varepsilon_z \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) \right\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \leq C\, C_\beta\, \varepsilon^\beta \left(\int_{|z|>R} \langle z \rangle^{-2(N_\beta - k)} dz \right)^{1/2}.$$

In the following, we will use the notation

$$\phi^\varepsilon_{R,<} := \mathcal{J}\left[g^\varepsilon_z \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) = \mathcal{B}_\varepsilon^{-1}\left(\mathrm{Id}_{|z|<R} \mathcal{B}^\varepsilon[\phi^\varepsilon](z)\right). \tag{C.1}$$

Remark C.3. Lemma C.2 can be used in different manners.

1. If $\beta > 0$, then $\mathcal{J}[g^\varepsilon_z \chi(|z|/R)](\phi^\varepsilon)$ approximates ϕ^ε in $L^2(\mathbb{R}^d)$ as ε goes to 0 in any space $\Sigma^k_\varepsilon(\mathbb{R}^d)$ with $k \in \mathbb{N}$ such that $N_\beta > k + d$, and uniformly with respect to $R > R_\beta$.
2. If $\beta \geq 0$ (including $\beta = 0$), then the same approximation holds by letting R go to $+\infty$, and it is uniform with respect to ε. In particular, when $\beta = 0$ we have

$$\limsup_{\varepsilon \to 0} \left\| \phi^\varepsilon - \mathcal{J}\left[g^\varepsilon_z \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) \right\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \leq C R^{-(N_\beta - k - d)}.$$

Proof. We set

$$r^\varepsilon(x) = (2\pi\varepsilon)^{-d} \int_{|z|\geq R} \langle g^\varepsilon_z, \varphi^\varepsilon \rangle g^\varepsilon_z(x) dz$$

and consider $k \in \mathbb{N}$. For $R > R_\beta$, $\alpha, \gamma \in \mathbb{N}^d$ with $|\alpha| + |\gamma| = k$, we have

$$\|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} \leq (2\pi\varepsilon)^{-2d} \int_{\mathbb{R}^d} \int_{|z|>R} \int_{|z'|>R} \langle g_z^\varepsilon, \varphi^\varepsilon \rangle \, \overline{\langle g_{z'}^\varepsilon, \varphi^\varepsilon \rangle} g^{\alpha,\gamma}_{\varepsilon,z}(x) \, \overline{g^{\alpha,\gamma}_{\varepsilon,z'}(x)} \, dx \, dz \, dz'.$$

where

$$g^{\alpha,\gamma}_{\varepsilon,z} = x^\alpha (\varepsilon D_x)^\gamma g_z^\varepsilon = \mathrm{WP}_z^\varepsilon \left((q + \sqrt{\varepsilon} y)^\alpha (p + \sqrt{\varepsilon} D_y)^\gamma g_0 \right), \quad z = (q,p). \tag{C.2}$$

We will use that for all $n \in \mathbb{N}$, there exists $c_{n,k} > 0$ such that for all $z \in \mathbb{R}^{2d}$

$$\|g^{\alpha,\gamma}_{\varepsilon,z}\|_{\Sigma^n} \leq c_{n,k} \langle z \rangle^k. \tag{C.3}$$

By (3.4), we obtain

$$\begin{aligned} &\|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} \\ &\quad \leq C_\beta^2 \, \varepsilon^{2\beta} \, (2\pi\varepsilon)^{-d} \int_{|z|>R} \int_{|z'|>R} \langle z \rangle^{-N_\beta} \langle z' \rangle^{-N_\beta} \, W[g^{\alpha,\gamma}_{\varepsilon,z}, g^{\alpha,\gamma}_{\varepsilon,z'}] \left(\frac{z - z'}{\sqrt{\varepsilon}} \right) dz \, dz'. \end{aligned}$$

Besides, by (3.5), there exists a constant $C'_{n,k}$ such that

$$\left| W[g^{\alpha,\gamma}_{\varepsilon,z}, g^{\alpha,\gamma}_{\varepsilon,z'}](\zeta) \right| \leq C'_{n,k} \, \langle \zeta \rangle^{-n} \langle z \rangle^k \langle z' \rangle^k.$$

We deduce the existence of $c > 0$ such that

$$\begin{aligned} \|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} &\leq c \, C_\beta^2 \, \varepsilon^{2\beta} \, \varepsilon^{-d} \int_{|z|>R} \int_{|z'|>R} \langle z \rangle^{-N_\beta + k} \langle z' \rangle^{-N_\beta + k} \left\langle \frac{z - z'}{\sqrt{\varepsilon}} \right\rangle^{-n} dz dz' \\ &\leq c \, C_\beta^2 \, \varepsilon^{2\beta} \int_{|z|>R} \int \langle z \rangle^{-N_\beta + k} \langle z + \sqrt{\varepsilon} \zeta \rangle^{-N_\beta + k} \langle \zeta \rangle^{-n} dz d\zeta. \end{aligned}$$

Since $-N_\beta + k \leq 0$, Peetre inequality (3.6) gives

$$\langle z + \sqrt{\varepsilon} \zeta \rangle^{-N_\beta + k} \leq 2^{\frac{N_\beta - k}{2}} \langle \sqrt{\varepsilon} \zeta \rangle^{N_\beta - k} \langle z \rangle^{-N_\beta + k} \leq 2^{\frac{N_\beta - k}{2}} \langle \zeta \rangle^{N_\beta - k} \langle z \rangle^{-N_\beta + k},$$

by restricting ourselves to $\varepsilon \leq 1$. Therefore, there exists a constant $c > 0$ such that

$$\|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} \leq c \, C_\beta^2 \, \varepsilon^{2\beta} \left(\int_{\mathbb{R}^{2d}} \langle \zeta \rangle^{-n + N_\beta - k} d\zeta \right) \left(\int_{|z|>R} \langle z \rangle^{-2(N_\beta - k)} dz \right)$$

and we conclude the proof by choosing $n = N_\beta + k + 2d + 1$. □

Let us conclude this section by some examples.

Example C.4.
1. Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$ such that $\phi^\varepsilon = \mathrm{Id}_{|x| \leq M} \phi^\varepsilon$ and $\mathcal{F}^\varepsilon \phi^\varepsilon = \mathrm{Id}_{|\xi| \leq M} \mathcal{F}^\varepsilon \phi^\varepsilon$ for some $M > 0$. Then, $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localised at any scale $\beta \geq 0$.
2. Let $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $z_0 = (q_0, p_0) \in \mathbb{R}^{2d}$. Then, the family $(\mathrm{WP}^\varepsilon_{z_0}(\varphi))_{\varepsilon>0}$ is frequency localized at the scale β for any $\beta \geq 0$.
3. Let $a \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ and $S \in \mathcal{C}^\infty(\mathbb{R}^d)$. Then, the family $(\mathrm{e}^{\frac{i}{\varepsilon} S(x)} a)_{\varepsilon>0}$ is frequency localized at the scale β for any $\beta \geq 0$.

An important consequence is related with the notion of compacity and of ε-oscillation that are often considered in semi-classical analysis. We recall that the uniformly bounded family $(\phi^\varepsilon)_{\varepsilon>0}$ is said to be compact if

$$\limsup_{\varepsilon \to 0} \int_{|x|>R} |\phi^\varepsilon(x)|^2 dx \underset{R \to +\infty}{\longrightarrow} 0.$$

It is said to be ε-oscillating when

$$\limsup_{\varepsilon\to 0}\int_{|\xi|>\frac{R}{\varepsilon}}|\widehat{\phi}^\varepsilon(\xi)|^2 d\xi \underset{R\to+\infty}{\longrightarrow} 0,$$

or, equivalently, when its ε-Fourier transform $(\mathcal{F}^\varepsilon\phi^\varepsilon)_{\varepsilon>0}$ is compact. Therefore, a family which is simultaneously compact and ε-oscillatory can be approached by frequency-localized families, uniformly in ε. In view of its importance, we terminate this paragraph by discussing the case (1) of bounded families that are compactly supported and have ε-Fourier transform compactly supported. The two other ones are treated in the Appendix.

Analysis of case (1) in Example C.4. Without loss of generality, we may assume $M>1$. We start with the observation that by assumption, for all $z=(q,p)\in\mathbb{R}^{2d}$

(C.4)

$$|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2\le(2\pi\varepsilon)^{-d}\|g_z^\varepsilon 1_{|x|<M)}\|_{L^2}^2=(2\pi\varepsilon)^{-d}\int_{|x|\le M}\mathrm{e}^{-\frac{|x-q|^2}{\varepsilon}}dx\le(2\pi\varepsilon)^{-d}\,M^d\mathrm{e}^{-\frac{|q|^2}{\varepsilon}+\frac{2}{\varepsilon}M|q|}.$$

Similarly, by Plancherel theorem,

(C.5)

$$|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2\le(2\pi\varepsilon)^{-d}\|\mathcal{F}_\varepsilon g_z^\varepsilon 1_{|\xi|<M)}\|_{L^2}^2=(2\pi\varepsilon)^{-d}\int_{|\xi|\le M}\mathrm{e}^{-\frac{|\xi-p|^2}{\varepsilon}}d\xi\le(2\pi\varepsilon)^{-d}\,M^d\mathrm{e}^{-\frac{|p|^2}{\varepsilon}+\frac{2}{\varepsilon}M|p|}.$$

We now consider for $n\in\mathbb{N}$, $|z|>4M^2$ and $\beta>0$, the quantity $\varepsilon^{-\beta}|z|^{2n}|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2$.

(i) If $|q|>2M^2$ and $|p|>2M^2$, then we find constants $C,C'>0$ such that

$$\begin{aligned}\varepsilon^{-\beta}|z|^{2n}|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2&\le C\,\varepsilon^{-\beta}(|q|^{2n}+|p|^{2n})|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2\\&\le C'\,M^d\varepsilon^{-\beta-d}\left(|q|^{2n}\mathrm{e}^{-\frac{|q|^2}{\varepsilon}+\frac{2}{\varepsilon}M|q|}+|p|^{2n}\mathrm{e}^{-\frac{|p|^2}{\varepsilon}+\frac{2}{\varepsilon}M|p|}\right),\end{aligned}$$

where we have used (C.4) and (C.5). The estimate comes from the observation that the right-hand side converges to 0 uniformly in ε on the set $\{|q|>2M^2\}\cap\{|p|>2M^2\}$.

(ii) If $|q|\le 2M^2$, then necessarily $|p|>2M^2$. We follow the same line of discussion and write

$$\varepsilon^{-\beta}|z|^{2n}|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2\le C\varepsilon^{-\beta}(M^{4n}+|p|^{2n})|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2.$$

We then use (C.5) to obtain

$$\varepsilon^{-\beta}|z|^{2n}|\mathcal{B}^\varepsilon[\phi^\varepsilon](z)|^2\le C\varepsilon^{-\beta-d}(M^{4n}+|p|^{2n})M^d\mathrm{e}^{-\frac{|p|^2}{\varepsilon}+\frac{2}{\varepsilon}M|p|},$$

and conclude similarly.

(iii) If $|p|\le M^2$, then necessarily $|q|>2M^2$, and we argue as in the preceding step exchanging the roles of p and q.

This terminates the proof. □

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