Initial Value Representations

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Introduction

The time-dependent Schrödinger equation

$$i\varepsilon \frac{d}{dt}\psi^\varepsilon = H^\varepsilon(t)\psi^\varepsilon, \qquad \psi(0) = \psi_0 \in L^2(\mathbb{R}^d) \tag{0.1}$$

needs little motivation. It has proven to be fundamental for the understanding of an abundant number of phenomena ranging from the classical double-slit experiment to reaction dynamics.

The subject of this dissertation is the semiclassical approximation of the propagator of (0.1) by a class of global Fourier Integral Operators (FIOs) with complex valued phase, which are known as Initial Value Representations (IVRs) in the chemical literature. The central result is formulated in Theorem 8.1. It is shown that Initial Value Representations approximate the unitary propagator associated to (0.1) in the uniform operator norm up to an error of order one in the semiclassical parameter ε. Moreover, corrections are presented, which improve the error bound to arbitrary order in ε and a slightly weaker result for the Ehrenfest-timescale is given.

Central intermediate results are the Calderón-Vaillancourt-like Theorems 4.11 and 5.4, which establish the boundedness of FIOs as operators from $L^2(\mathbb{R}^d)$ into itself and Proposition 7.3, which gives an asymptotic expansion for the composition of Weyl-quantised pseudodifferential operators (PDOs) and FIOs.

Part of the result has been published earlier in [RS08] and [SR08]. This work is generalised in two aspect. First, the class of accessible FIOs is extended from the Herman-Kluk propagator to more general IVRs. Second, the restriction to Schrödinger operators is alleviated and the result holds for general PDOs with subquadratic symbols.

Organisation of the dissertation

The dissertation is split into three parts: The first part will discuss aspects directly related to (0.1) and H^ε. We will recall the definition of Weyl-quantised PDOs and central results on them. Moreover, the existence of a unitary propagator associated to (0.1) is shown for the special case of PDOs with subquadratic symbols, a result which is known and contained as an exercise in [Rob87]. We present a new proof, which is inspired by the classical Faris-Lavine argument. The first part closes with some results on the canonical transformations associated to subquadratic symbols.

The second part is devoted to the Fourier Integral Operators under consideration. We present results, which show that they primarily act along the canonical transformation they are associated with and explain how the heuristic idea of an "overcomplete basis of coherent states" is related to the FIOs. Moreover, continuity result between Schwartz-spaces are shown and an ε-independent bound for the norm of FIOs as operators between L^2-spaces is established.

The last part connects the Fourier Integral Operators with (0.1). We give an asymptotic expansion of the composition of PDOs and FIOs and investigate the time-derivative of FIOs. These results are combined to the main Theorem on the approximation of unitary propagators by IVRs. The part is concluded with the presentation of some proof-of-concept computations.

A heuristic motivation for Initial Value Representations

Equations of type (0.1) arise in a variety of situations. In its most prominent form, ε equals the quantum of action $\hbar$, and the Hamilton operator H^ε is of the Schödinger form

$$H^\varepsilon = -\frac{\varepsilon^2}{2}\Delta + V(x) \tag{0.2}$$

for some potential V depending on the physical system. This classical Schrödinger equation is considered as the fundamental equation of non-relativistic quantum physics and is the basis for all applications in this field.

However, there are situations where the parameter ε has a different meaning. One important example is the computation of the single-state dynamics of molecules in the Born-Oppenheimer approximation, compare [ST01]. In this case, ε equals square root of the ratio of the electron and average nuclear mass of the molecule and its order of magnitude is approximately 10^{-3} to 10^{-2}. The ε in front of the time-derivative comes from the transformation to the time-unit $t_{\mathrm{BO}} = t_{\mathrm{phys}}/\varepsilon$. This "distinguished limit" ([Col68]) is necessary to work on timescales on which the nuclei show a nontrivial movement.

Solving (0.1) still poses a challenging problem to today's scientists. The particular difficulty lies in the nature of its solution. The wavefunction ψ is a complex-valued function on the configuration space $\mathbb{R}^d$, whose dimension is determined by the number of degrees of freedom of the system. Even for simple systems this dimension is usually prohibitive. Therefore one aims at approximate solutions to (0.1).

A very profitable approach in this respect is the semiclassical treatment of the system. It is common knowledge and experience that quantum dynamics reduces to classical mechanics for large energies and frequencies. Between the extremes of pure quantum behavior and classical mechanics, there is a regime, in which classical quantities can be used to describe the quantum behavior of the system. Many well-established methods like the WKB-ansatz and the Wigner method belong to this category of approximations. The principle idea is the following: if one can construct a function $\psi^\varepsilon_{\mathrm{sc}}$, which fulfills $\psi^\varepsilon = \psi^\varepsilon_{\mathrm{sc}} + O(\varepsilon)$ for small ε, one can hope that $\psi^\varepsilon_{\mathrm{sc}}$ is still a good approximation for the value of ε given by the application.

In the chemical physics community, the so-called Initial Value Representations (IVRs) were developed and proved to be a successful method for the treatment of molecular dynamics, see e.g. [Kay07]. The distinctive feature of IVRs is that they tackle the unitary propagator $U(t,s)$ of (0.1), whereas methods like the WKB or the Wigner-method only provide approximations for one specific initial datum, see e.g. [SMM03]. Moreover, they do not show phenomena like the breakdown of the WKB-method at turning points.

For a heuristic motivation, we specialise to Hamiltonians of the form (0.2), restrict to one-dimensional problems and start with the identity

$$\psi(x) = \frac{1}{2\pi\varepsilon}\int_{T^*\mathbb{R}} g^\varepsilon_{(q,p)}(x)\langle g^\varepsilon_{(q,p)}, \psi\rangle_{L^2(\mathbb{R})}\, dq\, dp, \tag{0.3}$$

where

$$g^\varepsilon_{(q,p)}(x) = \frac{1}{(\pi\varepsilon)^{1/4}} e^{-(x-q)^2/2\varepsilon} e^{ip(x-q)/\varepsilon} \tag{0.4}$$

denotes the coherent state centered at (q,p) in the phase space $T^*\mathbb{R}$. Within the chemical community, identity (0.3) is known as an "expansion in the overcomplete basis of coherent states". A more satisfactory explanation will be provided in Section 4.1.

Applying the unitary group of (0.1) to expression (0.3), one gets the formal equality

$$\left(e^{-\frac{i}{\varepsilon}H^\varepsilon t}\psi_0^\varepsilon\right)(x) = \frac{1}{2\pi\varepsilon}\int_{T^*\mathbb{R}} \left(e^{-\frac{i}{\varepsilon}H^\varepsilon t}g^\varepsilon_{(q,p)}\right)(x)\langle g^\varepsilon_{(q,p)}, \psi_0^\varepsilon\rangle_{L^2(\mathbb{R})}\, dq\, dp. \tag{0.5}$$

Hence, one expects an approximation to the solution of (0.1), if approximate expressions for the time-evolution of coherent states are used in (0.5). Such expressions have been studied for a long time. They rely on the classical flow $(q(t,q,p), p(t,q,p))$ which arises from Newton's equation of motion

$$\begin{aligned} \frac{d}{dt}q(t,q,p) &= p(t,q,p), && q(0,q,p) = q \\ \frac{d}{dt}p(t,q,p) &= -V'(q(t,q,p)), && p(0,q,p) = p \end{aligned}$$

and are in the simplest case given by

$$\begin{aligned} \left(e^{-\frac{i}{\varepsilon}H^\varepsilon t}g^\varepsilon_{(q,p)}\right)(x) \approx \frac{1}{(\pi\varepsilon)^{1/4}} &\left[(\partial_q q(t,q,p) + i\partial_p q(t,q,p))\right]^{-\frac{1}{2}} \\ &\times e^{\frac{i}{\varepsilon}S(t,q,p)}\, e^{-\Theta(t,q,p)(x-q(t,q,p))^2/2\varepsilon}\, e^{ip(t,q,p)(x-q(t,q,p))/\varepsilon}, \end{aligned} \tag{0.6}$$

where

$$\Theta(t,q,p) = -i\left(\partial_q p(t,q,p) + i\partial_p p(t,q,p)\right)\left(\partial_q q(t,q,p) + i\partial_p q(t,q,p)\right)^{-1}$$

encodes the time-dependent width of the propagated coherent state and

$$S(t,q,p) = \int_0^t \left[\tfrac{1}{2}p(\tau,q,p)^2 - V\left(q(\tau,q,p)\right)\right]\, d\tau$$

denotes the classical action of the trajectory $\tau \mapsto (q(t,q,p), p(t,q,p))$. The expression was formally established in [Hel75b] and baptised "Thawed Gaussian Approximation". Rigorous results and more conceptual derivations can be found in [Hag80], [Hag98] and [CR97].

Combining (0.3) and (0.5) we obtain the so-called Thawed Gaussian Initial Value Representation, which is formally given as

$$\left(e^{-\frac{i}{\varepsilon}H^\varepsilon t}\psi_0^\varepsilon\right)(x) \approx (2\pi\varepsilon)^{-3/2}\int_{\mathbb{R}^3} e^{\frac{i}{\varepsilon}\Phi(t,x,y,q,p;\Theta)}u(t,q,p)\varphi(y)\, dq\, dp\, dy \tag{0.7}$$

where the *phase function* Φ reads

$$\begin{aligned} \Phi(t,x,y,q,p;\Theta) := {}& S(t,q,p) + p(t,q,p)(x - q(t,q,p)) - p(y-q) \\ &+ i\Theta(t,q,p)(x-q(t,q,p))^2/2 + i(y-q)^2/2 \end{aligned} \tag{0.8}$$

and the *symbol* u is given by

$$u(t,q,p) = 2\left[(\partial_q q(t,q,p) + i\partial_p q(t,q,p))\right]^{-\frac{1}{2}}.$$

In the mathematical literature, expressions like (0.7) are known as Fourier Integral Operators with complex valued phase function. From the viewpoint of this theory, the central characteristic of Φ is that its stationary points with respect to (q,p)

$$\Im\Phi(t,x,y,q_*,p_*;\Theta) = 0, \quad \partial_{(q,p)}\Re\Phi(t,x,y,q_*,p_*;\Theta) = 0$$

are determined by

$$q_* = y, \quad x = q(t, q_*, p_*), \tag{0.9}$$

i.e. the phase is stationary if and only if there is a classical trajectory $t \mapsto q(t, y, p_*)$, which connects the points x and y and that the phase fulfills the non-degeneracy condition

$$\det \begin{pmatrix} \partial_{xy}\Phi & \partial_{x\theta}\Phi \\ \partial_{y\theta}\Phi & \partial_{\theta\theta}\Phi \end{pmatrix} \neq 0$$

on the set of stationary points. A few lines of computation reveal that

$$\det \begin{pmatrix} \partial_{xy}\Phi & \partial_{x\theta}\Phi \\ \partial_{y\theta}\Phi & \partial_{\theta\theta}\Phi \end{pmatrix} \geq (\Re\Theta(t, q, p))^{\frac{1}{2}} . \tag{0.10}$$

Hence, considering (0.9) and (0.10) there is little reason why Θ should have the specific form derived from (0.6). Indeed, the most successful IVR, the so-called Herman-Kluk propagator, which is given by

$$\frac{1}{(2\pi\varepsilon)^{3/2}} \int_{\mathbb{R}^3} e^{\frac{i}{\varepsilon}\Phi_{\mathrm{HK}}(t,x,y,q,p)} u_{\mathrm{HK}}(t, q, p)\varphi(y)\, dq\, dp\, dy,$$

with

$$\begin{aligned} \Phi_{\mathrm{HK}}(t, x, y, q, p) = {} & S(t, q, p) + p(t, q, p)(x - q(t, q, p)) - p(y - q) \\ & + i(x - q(t, q, p))^2/2 + i(y - q)^2/2 \end{aligned}$$

and

$$u_{\mathrm{HK}}(t, q, p) = [\partial_q q(t, q, p) - i\partial_p q(t, q, p) + i\partial_q p(t, q, p) + \partial_p p(t, q, p)]^{\frac{1}{2}}$$

does not change the width of the coherent states during the time-evolution. Our main result will be concerned with a general class of such FIOs which includes both the TGA-IVR and the Herman-Kluk propagator as special cases.

At the end of this introduction, we want to point the reader to further discussions of the existing literature. In the first chapter of Part II we give a short discussion of the classical approach to global Fourier Integral Operators which gives some insight on the importance of conditions (0.9) and (0.10). A short history of Initial Value Representations is provided at the beginning of Part III followed by a presentation of prior results on the approximation of the propagator of (0.1) by Fourier Integral Operators.

A word on notation

Throughout this work, we will mostly use standard symbols and notations such as $C^\infty(\mathbb{R}^d)$ for the complex-valued smooth functions on $\mathbb{R}^d$ and $\mathcal{S}(\mathbb{R}^d)$ for the Schwartz functions on $\mathbb{R}^d$. Moreover, we note that our scalar products are linear with respect to the second argument, i.e.

$$\langle \alpha\varphi|\beta\psi\rangle_{L^2(\mathbb{R}^d)} = \overline{\alpha}\beta \, \langle\varphi|\psi\rangle_{L^2(\mathbb{R}^d)} , \qquad \varphi, \psi \in L^2(\mathbb{R}^d)$$

and that we chose the normalisation

$$(\mathcal{F}^\varepsilon\psi)(\xi) = (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} e^{-\frac{i}{\varepsilon}\xi\cdot x}\psi(x)\, dx, \qquad \psi \in \mathcal{S}(\mathbb{R}^d) \tag{0.11}$$

for the Fourier-transform to make it unitary on $L^2(\mathbb{R}^d)$.

One main non-standard notation concerns quadratic forms. For a complex symmetric matrix $A \in \mathbb{C}^{d\times d}$, i.e. $A = A^\dagger = \overline{A}^*$ and a vector $x \in \mathbb{R}^d$, we use the shorthand notation

$$Ax^2 := x^\dagger Ax = x \cdot Ax.$$

A second pitfall concerns derivatives of vector valued functions. For a mapping $f \in C^1(\mathbb{R}^d, \mathbb{R}^d)$ we denote by $f_x(x) = (\partial_x f)(x)$ the transpose of the Jacobian, i.e.

$$\left(f_x(x)\right)_{jk} = (\partial_{x_j} f_k)(x) = \frac{\partial f_k}{\partial x_j}(x).$$

This definition is useful because we consider all vectors $v \in \mathbb{R}^d$ as column vectors, but it leads to somewhat unusual identities when chain and product rules are applied. For example, we have

$$\begin{aligned} \partial_x(f \cdot g)(x) &= f_x(x)g(x) + g_x(x)f(x) \\ \partial_x f(g(x)) &= g_x(x)f_x(g(x)) \qquad \text{and} \\ \partial_x(Af(x)) &= f_x(x)A \end{aligned}$$

for mappings $f, g \in C^1(\mathbb{R}^d, \mathbb{R}^d)$ and symmetric matrices $A \in \mathbb{C}^{d\times d}$. Finally, we will meet some special differential operators for which we use the convention

$$\frac{1 - i\varepsilon\Phi_x(x)\cdot\nabla_x}{1 + |\Phi_x(x)|^2} := \left(1 + |\Phi_x(x)|^2\right)^{-1} \left(1 - i\varepsilon\Phi_x(x)\cdot\nabla_x\right).$$

All other notations with hints to their first appearance are collected in Section 9 in the appendix.

Part I

The Problem

1 The Schrödinger equation

The insight that quantum mechanics is the fundamental theory which simplifies to classical mechanics in macroscopic systems is undisputed. However, in practical applications, the physically correct Hamilton operator H^ε is a priori unknown and has to be derived from the system under consideration. This modelling process is usually a two-step procedure. First, one chooses a Hamilton function $h(x,\xi)$, later on called the symbol, based on a classical understanding of the system. In the step of quantisation one associates a linear operator $H^\varepsilon = \mathrm{op}^\varepsilon(h)$ in $L^2(\mathbb{R}^d)$ to h such that the correspondances

$$\begin{aligned} \mathrm{op}^\varepsilon(x_j)\varphi(x) &= x_j\varphi(x) \\ \mathrm{op}^\varepsilon(\xi_j)\varphi(x) &= -i\varepsilon\partial_{x_j}\varphi(x) \quad \text{and} \\ \mathrm{op}^\varepsilon(1)\varphi(x) &= \varphi(x) \end{aligned}$$

hold and the map $h \to \mathrm{op}^\varepsilon(h)$ is linear. One class of quantisations is based on the Fourier-transformation. If $\psi \in \mathcal{S}(\mathbb{R}^d)$, we have the identities

$$\begin{aligned} \psi(x) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\psi(x')\,dx'\right]d\xi \\ x\psi(x) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}x'\psi(x')\,dx'\right]d\xi \quad \text{and} \\ -i\varepsilon\partial_{x_j}\psi(x) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\xi_j\psi(x')\,dx'\right]d\xi. \end{aligned}$$

Hence, a class of quantisations is formally given as

$$\mathrm{op}^\varepsilon_\sigma(h) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}h(\sigma x + (1-\sigma)x',\xi)\psi(x')\,dx'\,d\xi, \quad \psi \in \mathcal{S}(\mathbb{R}^d) \tag{1.1}$$

where σ ranges in $[0,1]$. The difference between different values of σ boils down to the treatment of the symbol $x_j\xi_j$, which is quantised to

$$\mathrm{op}^\varepsilon_\sigma(x_j\xi_j) = \sigma\left[x_j \circ \left(-i\varepsilon\partial_{x_j}\right)\right] + (1-\sigma)\left[\left(-i\varepsilon\partial_{x_j}\right)\circ x_j\right],$$

i.e. $\sigma = 0$ yields the *pq*-quantisation, whereas $\sigma = 1$ results in the *qp*-quantisation. In Section 4.1 we will meet the Wick and Anti-Wick quantization schemes, which are based on a different concept.

1.1 Weyl-quantisation and symbol classes

In the context of quantum mechanics, the Weyl-quantisation, which arises for $\sigma = \frac{1}{2}$ is most natural. For $h \in \mathcal{S}(\mathbb{R}^{2d})$ and $\psi \in \mathcal{S}(\mathbb{R}^d)$ it is given by the absolutely convergent integral

$$\left(\mathrm{op}^\varepsilon(h)\psi\right)(x) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}h\left(\frac{x+x'}{2},\xi\right)\psi(x')\,d\xi\,dx'. \tag{1.2}$$

For the extension to more general symbols, several approaches can be taken. For instance, one can use the Wigner function

$$\begin{aligned} \mathcal{W} : \mathcal{S}(\mathbb{R}^d) \times \mathcal{S}(\mathbb{R}^d) &\to \mathcal{S}(\mathbb{R}^{2d}) \\ (\varphi, \psi) &\mapsto \mathcal{W}^\varepsilon[\varphi, \psi](q,p) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{iy\cdot p} \varphi\left(q - \tfrac{\varepsilon}{2} y\right) \overline{\psi\left(q + \tfrac{\varepsilon}{2} y\right)}\, dy \end{aligned} \tag{1.3}$$

and the relation

$$\langle \overline{\psi} | \mathrm{op}^\varepsilon(h)\varphi \rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} \mathcal{W}^\varepsilon[\varphi, \overline{\psi}](q,p) h(q,p)\, dq\, dp, \quad \varphi, \psi \in \mathcal{S}(\mathbb{R}^d). \tag{1.4}$$

Now the Wigner-transform is the Fourier transform of the Schwartz class function

$$(q,y) \mapsto \varphi\left(q - \tfrac{\varepsilon}{2} y\right) \overline{\psi\left(q + \tfrac{\varepsilon}{2} y\right)}$$

with respect to the second variable and thus continuous from $\mathcal{S}(\mathbb{R}^d) \times \mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^{2d})$. This shows that the left hand side of (1.4) is a continuous linear form in $\psi \in \mathcal{S}(\mathbb{R}^d)$, which allows for the interpretation

$$\mathrm{op}^\varepsilon(h) : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d). \tag{1.5}$$

Reading the right hand side of (1.4) as a dual pairing between $h \in \mathcal{S}(\mathbb{R}^{2d}) \subset \mathcal{S}'(\mathbb{R}^{2d})$ and $\mathcal{W}[\varphi, \overline{\psi}] \in \mathcal{S}(\mathbb{R}^{2d})$ and keeping the sense (1.5), one can then extend the admissible symbols to $h \in \mathcal{S}'(\mathbb{R}^{2d})$ by defining the pairing between $\mathrm{op}^\varepsilon(h)\varphi$ and ψ by the right-hand side of (1.4).

However, we will hardly be able to associate a classical mechanical system to a "Hamilton distribution" and do not need such a general notion of symbols for our application. Moreover, (1.2) provides a much more explicit expression for the operator than (1.4) does. Therefore we restrict ourselves to symbols, which allow for the definition of Weyl-quantisation in terms of explicit oscillatory integrals. The following presentation is based on that of [Mar02].

The problem of generalising (1.2) as an ordinary Lesbegue-integral lies in the convergence of the ξ-integral. The main tool to circumvent this difficulty is the operator

$$\begin{aligned} L_{x'} : C^\infty(\mathbb{R}^d) &\to C^\infty(\mathbb{R}^d) \\ \varphi &\mapsto L_{x'}\varphi = \frac{1 + i\varepsilon\xi \cdot \nabla_{x'}}{1 + |\xi|^2} \varphi. \end{aligned} \tag{1.6}$$

$L_{x'}$ fulfills

$$L_{x'} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} = e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}.$$

Hence, by integration by parts in y (1.2) equals

$$(2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} \left(L_{x'}^\dagger\right)^k \left[h\left(\frac{x+x'}{2}, \xi\right) \psi(x') \right]\, dx'\, d\xi,$$

for any $k \in \mathbb{N}$, where

$$L_{x'}^\dagger = \frac{1 - i\varepsilon\xi \cdot \nabla_{x'}}{1 + |\xi|^2}$$

denotes the adjoint of $L_{x'}$ with respect to the Banach-space structure on $L^2(\mathbb{R}^d)$, i.e.

$$\int_{\mathbb{R}^d} (L_{x'}\varphi)(x')\psi(x')\, dx' = \int_{\mathbb{R}^d} \varphi(x') \left(L_{x'}^\dagger \psi\right)(x')\, dx' \qquad \forall \psi, \varphi \in \mathcal{S}(\mathbb{R}^d).$$

Moreover, by Lemma 10.2 in the appendix, we have

$$\left|\left[\left(L_{x'}^{\dagger}\right)^{k}\varphi\right](x)\right| \leq \frac{C_k}{(1+|\xi|^2)^{k/2}}\sum_{|\alpha|\leq k}\left|\left(\partial_{x'}^{\alpha}\varphi\right)(x)\right|,$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$, where C_k depends only on k. Thus the integrations by parts convert the oscillatory behaviour in ξ of the integral into polynomial decay. We adapt the choice of our symbol classes to this methodology:

1.1 Definition (Symbol class). *Let* $\mathbf{m} = (m_j)_{1\leq j\leq J} \in \mathbb{R}^J$, $\mathbf{d} = (d_j)_{1\leq j\leq J} \in \mathbb{N}^J$ *and* $\rho \in [0,1]$. *We say that* $u^{\cdot} :]0,1] \times \mathbb{R}^{|\mathbf{d}|} \to \mathbb{C}^N$ *is a **symbol of class*** $S^{\rho}[\mathbf{m};\mathbf{d}]$, *if there is* $\varepsilon_0 \leq 1$, *such that* $u^{\varepsilon} \in C^{\infty}(\mathbb{R}^{|\mathbf{d}|};\mathbb{C}^N)$ *for all* $\varepsilon \leq \varepsilon_0$ *and*

$$M_k^{\mathbf{m}}[u] := \sup_{\varepsilon\leq\varepsilon_0}\max_{|\alpha|=k}\varepsilon^{k\rho}\sup_{z_j\in\mathbb{R}^{d_j}}\left|\left[\prod_{j=1}^{J}\langle z_j\rangle^{-m_j}\right]\partial_z^{\alpha}u^{\varepsilon}(z)\right| < \infty \tag{1.7}$$

for all $k \geq 0$, *where* $\langle z\rangle := \sqrt{1+|z|^2}$. *We extend this definition to any* $m_j \in \mathbb{R}\cup\{-\infty,+\infty\}$ *by setting for instance*

$$S^{\rho}[(+\infty,m_2,\dots,m_J);\mathbf{d}] = \bigcup_{m_1\in\mathbb{R}^{d_1}} S^{\rho}[(m_1,m_2\dots,m_J);\mathbf{d}] \qquad \textit{and}$$
$$S^{\rho}[(-\infty,m_2,\dots,m_J);\mathbf{d}] = \bigcap_{m_1\in\mathbb{R}^{d_1}} S^{\rho}[(m_1,m_2\dots,m_J);\mathbf{d}].$$

Moreover, we write $S[\mathbf{m};\mathbf{d}] := S^0[\mathbf{m};\mathbf{d}]$.

In particular, the growth of these symbols is only polynomial and can be compensated by the technique just explained. The smoothness is a tribute to a simple presentation as it allows to stay within the theory of Schwartz-spaces. To connect with the literature, we note that the symbol classes of Definition 1.1 coincide with the ones used in [Mar02] and [Rob87] and that we have $S^m_{0,0} = S[(0,m);(d,d)]$ with respect to the symbol classes $S^m_{\rho,\delta}$ used in [Hör85].

One defines (Compare Definitions 2.4.2 and 2.5.1 in [Mar02]):

1.2 Definition (Weyl-quantisation). *For* $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $h \in S[(+\infty,m);(d,d)]$ *and* $k > m+d$, *we define the **Weyl-quantisation*** $\mathrm{op}^{\varepsilon}(h)$ *of* h *as*

$$\left(\mathrm{op}^{\varepsilon}(h)\varphi\right)(x) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\left(L_{x'}^{\dagger}\right)^{k}\left[h\left(\frac{x+x'}{2},\xi\right)\varphi(x')\right]\,dx'\,d\xi.$$

The definition of oscillatory integrals via integration by parts with operators like (1.6) is a standard approach. We will follow the same strategy in Definitions 4.8 and 5.1 when we introduce our Fourier Integral Operators. An alternative possibility for the definition of oscillatory is presented in the first assertion of the following lemma. The second assertion shows the connection with the definition via the duality relation (1.4) sketched before.

1.3 Lemma. *Let* $h \in S[+\infty;2d]$.

1. *If* $\chi \in \mathcal{S}(\mathbb{R}^d)$ *with* $\chi(0)=1$, *we have*

$$\left(\mathrm{op}^{\varepsilon}(h)\varphi\right)(x) = \lim_{\lambda\to\infty}(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\chi(\xi/\lambda)h\left(\frac{x+x'}{2},\xi\right)\varphi(x')\,dx'\,d\xi.$$

2. $\mathrm{op}^\varepsilon(h)$ *fulfills* (1.4) *for any* $\varphi, \psi \in \mathcal{S}(\mathbb{R}^d)$.

Proof.

1. We choose m such that $h \in S[m; 2d]$ and $k > m + d$. We have

$$\begin{aligned}
&\mathrm{op}^\varepsilon(h)\varphi(x) \\
&= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} \left(L_{x'}^\dagger\right)^k \left[h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\right] dx'\,d\xi \\
&= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} \lim_{\lambda\to\infty} \chi(\xi/\lambda) \left(L_{x'}^\dagger\right)^k \left[h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\right] dx'\,d\xi \\
&= \lim_{\lambda\to\infty} (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\chi(\xi/\lambda) \left(L_{x'}^\dagger\right)^k \left[h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\right] dx'\,d\xi \\
&= \lim_{\lambda\to\infty} (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\chi(\xi/\lambda) h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\,dx'\,d\xi,
\end{aligned}$$

where the exchange of the integral and the limit is justified by dominated convergence.

2. Let $\chi \in \mathcal{S}(\mathbb{R}^d)$ with $\chi(0) = 1$ and $k > m + d$. Using dominated convergence and reverting the integrations by parts, we have

$$\begin{aligned}
&\left\langle \overline{\psi} \middle| \mathrm{op}^\varepsilon(h)\varphi \right\rangle_{L^2(\mathbb{R}^d)} \\
&= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} \left(L_{x'}^\dagger\right)^k \left[h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\right] dx'\,d\xi\;\psi(x)\,dx \\
&= \lim_{\lambda\to\infty} (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{3d}} \chi(\xi/\lambda) e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} h\left(\frac{x+x'}{2}, \xi\right)\varphi(x')\psi(x)\,d\xi\,dx\,dx' \\
&= \lim_{\lambda\to\infty} (2\pi)^{-d} \int_{\mathbb{R}^{3d}} \chi(\xi/\lambda) e^{i\xi\cdot\delta_x} h\left(\hat{x}, \xi\right) \varphi\left(\hat{x} - \tfrac{\varepsilon}{2}\delta_x\right) \psi\left(\hat{x} + \tfrac{\varepsilon}{2}\delta_x\right)\,d\delta_x\,d\xi\,d\hat{x} \\
&= \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} \chi(\xi/\lambda)\mathcal{W}^\varepsilon[\varphi, \overline{\psi}](\hat{x}, \xi) h\left(\hat{x}, \xi\right)\,d\xi\,d\hat{x},
\end{aligned}$$

where we used the orthogonal transformation defined by

$$\begin{pmatrix} x \\ x' \end{pmatrix} = \begin{pmatrix} \hat{x} + \varepsilon\delta_x/2 \\ \hat{x} - \varepsilon\delta_x/2 \end{pmatrix}.$$

As $\mathcal{W}^\varepsilon[\varphi, \overline{\psi}] \in \mathcal{S}(\mathbb{R}^{2d})$, the integral is absolutely convergent and an application of the dominated convergence theorem concludes the proof.

□

As indicated earlier, the symbols of Definition 1.1 allow to stay in the context of $\mathcal{S}(\mathbb{R}^d)$-theory:

1.4 Proposition ([Mar02], Theorem 2.5.3)**.** *Let* $h \in S[+\infty; 2d]$. *Then* $\mathrm{op}^\varepsilon(h)$ *is continuous from* $\mathcal{S}(\mathbb{R}^d)$ *to* $\mathcal{S}(\mathbb{R}^d)$.

1.2 Existence & uniqueness of solutions

With this basic comprehension for our Hamiltonians at hand, we turn to the existence and uniqueness of a propagator associated to

$$i\varepsilon\frac{d}{dt}\psi = \mathrm{op}^\varepsilon(h)\psi, \qquad \psi(0) = \psi_0 \in L^2(\mathbb{R}^d). \tag{1.8}$$

It is well-known that this question is intimately related to the selfadjointness of the Hamiltonian. Actually, in the case of a time-independent Hamilton operator, the existence of unique dynamics is equivalent to this property by Stone's Theorem. It is the distinctive feature of the Weyl-quantisation that classical Hamilton functions are quantised to candidates for self-adjoint operators:

1.5 Lemma. *Let $h \in S[+\infty; 2d]$ be a real symbol. Then $\mathrm{op}^\varepsilon(h)$ is symmetric on $\mathcal{S}(\mathbb{R}^d)$.*

Proof. The property is easily proved with help of the Wigner function:

$$\begin{aligned}\langle\varphi|\mathrm{op}^\varepsilon(h)\psi\rangle_{L^2(\mathbb{R}^d)} &= \int_{\mathbb{R}^{2d}} \mathcal{W}^\varepsilon[\varphi,\psi](q,p)h(q,p)\,dq\,dp \\ &= \int_{\mathbb{R}^{2d}} \overline{\mathcal{W}^\varepsilon[\psi,\varphi](q,p)}\,\overline{h(q,p)}\,dq\,dp \\ &= \overline{\langle\psi|\mathrm{op}^\varepsilon(h)\varphi\rangle_{L^2(\mathbb{R}^d)}} = \langle\mathrm{op}^\varepsilon(h)\varphi|\psi\rangle_{L^2(\mathbb{R}^d)}\,.\end{aligned}$$

□

To understand in which situations we can expect the essential self-adjointness of $\mathrm{op}^\varepsilon(h)$, we examine the case of one-dimensional Schrödinger operators

$$h(x,\xi) = \xi^2/2 + V(x), \quad V(x) \in C^\infty(\mathbb{R})$$

in more detail. The Faris-Lavine Theorem shows that a quadratic bound from below on the potential, i.e. $V(x) \geq -C_V\langle x\rangle^2$ for some $C_V > 0$ yields the essential selfadjointness of $\mathrm{op}^\varepsilon(h)$ on C_0^∞. The quadratic bound from below is the borderline case for essential selfadjointness. Theorems X.7 and X.9 in [RS75] show that the operator

$$H^\varepsilon = -\frac{\varepsilon^2}{2}\Delta - |x|^\alpha$$

is essentially self-adjoint on C_0^∞ if and only if $\alpha \leq 2$. A general result on pseudodifferential operators has to respect this situation, i.e. we have to put a quadratic bound from below on the symbol. Now $\mathrm{op}^\varepsilon(h)$ is essentially selfadjoint if and only if $-\mathrm{op}^\varepsilon(h)$ is essentially self-adjoint, so if the result shall apply both to h and $-h$, we have to assume

$$-C\langle(x,\xi)\rangle^2 \leq -h \quad \Rightarrow \quad h \leq C\langle(x,\xi)\rangle^2\,.$$

Hence, we are led to define

1.6 Definition (Subquadratic symbol)**.** *Consider a time-dependent family of real-valued symbols $h \in C^\infty(]-T,T[\times\mathbb{R}^{2d},\mathbb{C})$, $T \in \mathbb{R}\cup\{+\infty\}$. h is called* ***subquadratic****, if*

$$\sup_{-T<t<T}\ \sup_{(x,\xi)\in\mathbb{R}^{2d}} \left|\partial^\alpha_{(x,\xi)} h(t,x,\xi)\right| < \infty \tag{1.9}$$

for all $|\alpha| \geq 2$ *and*

$$\sup_{-T<t<T} \sup_{(x,\xi)\in\mathbb{R}^{2d}} \left|\partial^\alpha_{(x,\xi)}(\partial_t h)(t,x,\xi)\right| < \infty \tag{1.10}$$

for all $|\alpha| \geq 0$. *It is called* ***sublinear****, if* (1.9) *holds for all* $|\alpha| \geq 1$ *and* (1.10) *for all* $|\alpha| \geq 0$.

This definition naturally includes time-independent symbols $h(x,\xi)$ when they are considered as constant with respect to time.

1.2.1 Essential self-adjointness

This symbol class actually fulfills our expectations:

1.7 Proposition. *Let* $h^\varepsilon = h_0 + \varepsilon h_1 \in S[2;2d]$ *be a time-independent subquadratic symbol. There is* $\varepsilon_0 > 0$ *such that* $\mathrm{op}^\varepsilon(h^\varepsilon)$ *is essentially self-adjoint on* $\mathcal{S}(\mathbb{R}^d)$ *for all* $\varepsilon \leq \varepsilon_0$.

The result is contained as Exercise (IV-12) in [Rob87], where the existence of the propagator associated to $\mathrm{op}^\varepsilon(h^\varepsilon)$ is shown to deduce the essential self-adjointness of $\mathrm{op}^\varepsilon(h^\varepsilon)$. Here we present a proof, which follows the idea of the Faris-Lavine Theorem and uses the commutator theorem. In particular this proof also applies to matrix-valued symbols without change.

1.8 Theorem ([RS75], Theorem X.37)**.** *Let* N *be a self-adjoint operator with* $N \geq 1$ *in the sense of quadratic forms. Let* H *be a symmetric operator with domain* $\mathcal{D}(H)$*, which is a core for* N*. If there are* $C_1, C_2 > 0$ *such that*

$$\|H\varphi\| \leq C_1 \|N\varphi\| \qquad \text{and} \tag{1.11}$$

$$\left|\langle H\varphi|N\varphi\rangle_{L^2(\mathbb{R}^d)} - \langle N\varphi|H\varphi\rangle_{L^2(\mathbb{R}^d)}\right| \leq C_2 \left\|N^{\frac{1}{2}}\varphi\right\|^2 \tag{1.12}$$

for all $\varphi \in \mathcal{D}(H)$*,* H *is essentially self-adjoint on* $\mathcal{D}(H)$*.*

The operator N will be chosen as the sum of $\mathrm{op}^\varepsilon(h^\varepsilon)$ and a harmonic oscillator, such that we can apply Théorème III-4 in [Rob87]. This result uses a Gårding inequality to establish the essential self-adjointness of pseudodifferential operators with positive principal symbols and will provide the self-adjointness and the bound from below for the operator N:

1.9 Theorem ([Rob87], Théorème III-4)**.** *Let* $h_0, h_1 \in S[+\infty;2d]$ *be real symbols fulfilling* $h_0(x,\xi) \geq \gamma_0 > 0$ *for all* $(x,\xi) \in \mathbb{R}^{2d}$ *and*

$$\left|\partial^\alpha_{x,\xi} h_1(x,\xi)\right| \leq C_\alpha \left|h_0(x,\xi)\right| \qquad \forall x,\xi \in \mathbb{R}^d$$

for all $\alpha \in \mathbb{N}^{2d}$. *Then there is* $\varepsilon_0 > 0$ *such that* $\mathrm{op}^\varepsilon(h_0 + \varepsilon h_1)$ *is essentially self-adjoint on* $\mathcal{S}(\mathbb{R}^d, \mathbb{C})$ *for all* $\varepsilon \leq \varepsilon_0$. *Moreover,* $\mathrm{op}^\varepsilon(h_0 + \varepsilon h_1)$ *is semipositive, i.e. for every* $\delta > 0$ *there is* $\varepsilon_\delta > 0$ *such that*

$$\langle \mathrm{op}^\varepsilon(h_0 + \varepsilon h_1)\psi|\psi\rangle_{L^2(\mathbb{R}^d)} \geq (\gamma_0 - \delta) \|\psi\|^2_{L^2(\mathbb{R}^d)}$$

for all $\varepsilon \in]0, \varepsilon_\delta]$.

As a second result, we will use the Calderón-Vaillancourt Theorem, which concerns the boundedness of pseudodifferential operators between L^2-spaces:

1.10 Theorem (Calderón-Vaillancourt, [CV72])**.** *If $h \in S[0;2d]$, $\mathrm{op}^\varepsilon(h)$ can be uniquely extended to a continuous operator on $L^2(\mathbb{R}^d)$ with the ε-independent norm-bound*

$$\|\mathrm{op}^\varepsilon(h)\|_{L^2\to L^2} \leq C \sum_{|\alpha|\leq 2d+1} \|\partial^\alpha_{(x,\xi)} h\|_\infty .$$

The original work of Calderón and Vaillancourt only applies to the case $\varepsilon = 1$. However, a rescaling argument translates the result to the semiclassical setting. We will follow this idea later on in the proof of an analogue L^2-boundedness result for FIOs and detail the rescaling there.

Finally, we will need a very simple composition result for pseudodifferential operators for the treatment of the commutator. The reader who is familiar with pseudodifferential calculus will immediately recognise the rudiments of the Moyal-product:

1.11 Lemma. *Let $h \in S[+\infty;2d]$. We have*

$$\mathrm{op}^\varepsilon(x_j)\mathrm{op}^\varepsilon(h) = \mathrm{op}^\varepsilon\left(x_j h + \frac{i\varepsilon}{2}\partial_{\xi_j} h\right) \qquad \mathrm{op}^\varepsilon(h)\mathrm{op}^\varepsilon(x_j) = \mathrm{op}^\varepsilon\left(x_j h - \frac{i\varepsilon}{2}\partial_{\xi_j} h\right)$$
$$\mathrm{op}^\varepsilon(\xi_j)\mathrm{op}^\varepsilon(h) = \mathrm{op}^\varepsilon\left(\xi_j h - \frac{i\varepsilon}{2}\partial_{x_j} h\right) \qquad \mathrm{op}^\varepsilon(h)\mathrm{op}^\varepsilon(\xi_j) = \mathrm{op}^\varepsilon\left(\xi_j h + \frac{i\varepsilon}{2}\partial_{x_j} h\right)$$

as operators from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^d)$ and thus

$$[\mathrm{op}^\varepsilon(x_j), \mathrm{op}^\varepsilon(h)] = i\varepsilon\mathrm{op}^\varepsilon\left(\partial_{\xi_j} h\right) \qquad [\mathrm{op}^\varepsilon(\xi_j), \mathrm{op}^\varepsilon(h)] = -i\varepsilon\mathrm{op}^\varepsilon\left(\partial_{x_j} h\right)$$
$$[\mathrm{op}^\varepsilon(x_j^2), \mathrm{op}^\varepsilon(h)] = 2i\varepsilon\mathrm{op}^\varepsilon\left(x_j\partial_{\xi_j} h\right) \qquad [\mathrm{op}^\varepsilon(\xi_j^2), \mathrm{op}^\varepsilon(h)] = -2i\varepsilon\mathrm{op}^\varepsilon\left(\xi_j\partial_{x_j} h\right)$$

in the same sense.

The proof of these identities relies on integration by parts and is not presented here. With these preparations, we are now able to prove the essential self-adjointness.

Proof of Proposition 1.7. Because of the subquadraticity of h^ε, we can choose $c > 0$ and $b > 0$ such that

$$h_0(x,\xi) + c(x^2+\xi^2) + b > 0 \tag{1.13}$$

and

$$|h_1(x,\xi)| \leq \left|h_0(x,\xi) + c(x^2+\xi^2) + b\right| \qquad \forall x,\xi \in \mathbb{R}^d.$$

We set

$$N := \mathrm{op}^\varepsilon(h^\varepsilon) + 2c\,\mathrm{op}^\varepsilon\left(x^2+\xi^2\right) + b.$$

By Theorem 1.9 N is essentially selfadjoint on $\mathcal{S}(\mathbb{R}^d)$ with some lower bound δ_0 for $\varepsilon \leq \varepsilon_0$. As every positive constant is N-bounded with bound zero, we may increase b without changing ε_0 or δ_0 by the Kato-Rellich Theorem (Theorem X.12 in [RS75]). Hence we may assume $N \geq 1$ after an adjustment of b.

Using

$$AB^2 + B^2A = 2BAB + [B,[B,A]]$$

we have

$$\begin{aligned} N^2 &= (\mathrm{op}^\varepsilon(h^\varepsilon)+b)^2 + 4c^2\,\left[\mathrm{op}^\varepsilon\left(x^2+\xi^2\right)\right]^2 + 4bc\,\mathrm{op}^\varepsilon\left(x^2+\xi^2\right) \\ &\quad + 2c\left[\mathrm{op}^\varepsilon(h^\varepsilon)\mathrm{op}^\varepsilon\left(x^2+\xi^2\right) + \mathrm{op}^\varepsilon\left(x^2+\xi^2\right)\mathrm{op}^\varepsilon(h^\varepsilon)\right] \\ &= (\mathrm{op}^\varepsilon(h^\varepsilon)+b)^2 + P_1 + P_2 + B \end{aligned}$$

in the sense of quadratic forms on $\mathcal{S}(\mathbb{R}^d)$, where

$$\begin{aligned} P_1 := 4c\sum_{j=1}^d &\left[\mathrm{op}^\varepsilon(x_j)\left(\mathrm{op}^\varepsilon(h^\varepsilon) + c\mathrm{op}^\varepsilon\left(x^2+\xi^2\right)+b\right)\mathrm{op}^\varepsilon(x_j)\right] \\ + 4c\sum_{j=1}^d &\left[\mathrm{op}^\varepsilon(\xi_j)\left(\mathrm{op}^\varepsilon(h^\varepsilon) + c\mathrm{op}^\varepsilon\left(x^2+\xi^2\right)+b\right)\mathrm{op}^\varepsilon(\xi_j)\right], \end{aligned}$$

$$\begin{aligned} P_2 &:= 2c^2\sum_{j=1}^d\left[\mathrm{op}^\varepsilon(x_j)[\mathrm{op}^\varepsilon\left(x^2+\xi^2\right),\mathrm{op}^\varepsilon(x_j)] + \mathrm{op}^\varepsilon(\xi_j)[\mathrm{op}^\varepsilon\left(x^2+\xi^2\right),\mathrm{op}^\varepsilon(\xi_j)]\right] \\ &= -4i\varepsilon c^2\sum_{j=1}^d\left[\mathrm{op}^\varepsilon(x_j)\mathrm{op}^\varepsilon(\xi_j) - \mathrm{op}^\varepsilon(\xi_j)\mathrm{op}^\varepsilon(x_j)\right] = 4\varepsilon^2c^2 \end{aligned}$$

and

$$\begin{aligned} B &:= 2c\sum_{j=1}^d\left[\,[\mathrm{op}^\varepsilon(x_j),[\mathrm{op}^\varepsilon(x_j),\mathrm{op}^\varepsilon(h^\varepsilon)]] + [\mathrm{op}^\varepsilon(\xi_j),[\mathrm{op}^\varepsilon(\xi_j),\mathrm{op}^\varepsilon(h^\varepsilon)]]\right] \\ &= -2c\,\varepsilon^2\sum_{j=1}^d\mathrm{op}^\varepsilon\left(\left[\partial_{x_j}^2+\partial_{\xi_j}^2\right]h^\varepsilon\right). \end{aligned}$$

Taking (1.13) into account, we see that

$$\mathrm{op}^\varepsilon(h^\varepsilon) + c\mathrm{op}^\varepsilon\left(x^2+\xi^2\right) + b > 0$$

after an adjustment of b. Thus P_1 and P_2 are positive, whereas B can be extended to a bounded operator on $L^2(\mathbb{R}^d)$ by the Calderón-Vaillancourt Theorem 1.10.

Hence we have

$$\begin{aligned} &\|(\mathrm{op}^\varepsilon(h^\varepsilon)+b)\psi\|^2 = \left\langle(\mathrm{op}^\varepsilon(h^\varepsilon)+b)^2\psi\middle|\psi\right\rangle_{L^2(\mathbb{R}^d)} \\ &= \left\langle N^2\psi\middle|\psi\right\rangle_{L^2(\mathbb{R}^d)} - \langle(P_1+P_2)\psi|\psi\rangle_{L^2(\mathbb{R}^d)} - \langle B\psi|\psi\rangle_{L^2(\mathbb{R}^d)} \\ &\le (1+\|B\|)\,\|N\psi\|^2 \end{aligned}$$

as $N>1$ and thus

$$\|\mathrm{op}^\varepsilon(h^\varepsilon)\psi\| \le \|(\mathrm{op}^\varepsilon(h^\varepsilon)-b)\psi\| + b\,\|\psi\| \le (b+\sqrt{1+\|B\|})\,\|N\psi\|\,.$$

Moreover

$$\begin{aligned} \pm i\,[\mathrm{op}^\varepsilon(h^\varepsilon),N] &= \pm i\left[\mathrm{op}^\varepsilon(h^\varepsilon),\mathrm{op}^\varepsilon(h^\varepsilon) + 2c\,\mathrm{op}^\varepsilon\left(x^2+\xi^2\right)+b\right] \\ &= \pm 2ic\left[\mathrm{op}^\varepsilon(h^\varepsilon),\mathrm{op}^\varepsilon\left(x^2+\xi^2\right)\right] \\ &= \pm 4c\varepsilon\mathrm{op}^\varepsilon(g^\varepsilon) \end{aligned} \tag{1.14}$$

with

$$g^\varepsilon(x,\xi) = \sum_{j=1}^{d} \left[x_j \left(\partial_{\xi_j} h^\varepsilon\right)(x,\xi) - \xi_j \left(\partial_{x_j} h^\varepsilon\right)(x,\xi) \right].$$

As the derivatives of h^ε are sublinear, we can choose $d > 0$ such that

$$\pm 4c\varepsilon g^\varepsilon + d(h^\varepsilon + 2c(x^2 + \xi^2) + b) > 0,$$

which, after a possible increase of b and decrease of ε_0, ensures that

$$0 < \mathrm{op}^\varepsilon\left(\pm 4c\varepsilon g^\varepsilon + d(h^\varepsilon + 2c(x^2+\xi^2) + b)\right) = \pm 4c\varepsilon \mathrm{op}^\varepsilon(g^\varepsilon) + dN. \tag{1.15}$$

Combining (1.14) and (1.15) we have established that

$$\left| \langle [N, \mathrm{op}^\varepsilon(h^\varepsilon)]\, \psi | \psi \rangle_{L^2(\mathbb{R}^d)} \right| \le d \, \langle N\psi|\psi\rangle_{L^2(\mathbb{R}^d)}.$$

Thus $\mathrm{op}^\varepsilon(h^\varepsilon)$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d)$ by Theorem 1.8. □

1.2.2 The time-dependent case

In the time-dependent case no equivalence between existence of a unique solution and properties of the Hamiltonian is known. However, there are some results on sufficient conditions, see for example [Kat53] or [Yaj87]. The main focus of these results lies on minimal regularity and integrability assumptions with respect to t and x of the Hamiltonian. Considering Definition 1.6, it is clear that we do not aim in this direction here.

The main application of time-dependent Hamiltonians lies in the treatment of laser-pulses used for example in spectroscopy. In dipole approximation, such system are modelled by Hamiltonians of the form

$$H(t) = -\frac{\varepsilon^2}{2}\Delta + V(x) - F(t)\cos(\omega t)\rho(x)\cdot r_E,$$

where $F(t)$ is the envelope the laser-pulse with frequency ω, whereas $r_E \in \mathbb{R}^3$ is the direction of the electrical field of the laser and $\rho(x) \in C^\infty(\mathbb{R}^d, \mathbb{R}^3)$ is the dipole moment of the molecule, compare [CTDL06]. Thus, if $F(t)$ and $\varphi(t)$ are chosen smooth with respect to time and an spatial cutoff for the dipole-moment is introduced, this application is covered by Definition 1.6. Though not explicitly mentioned, the proof also applies to matrix-valued Hamiltonians for which the treatment of laser-pulses is much more interesting.

To connect to the presentation in Chapter X.12 in [RS75], we turn to the framework of contraction semigroups generated by a family of operators $A(t)$. The proof of existence of a propagator is extremely constructive. After an affine transformation of time, it is enough to consider the time-interval $[0,1]$. There, one defines

$$U_n(t,s) := \begin{cases} \exp\left(-(t-s)A\left(\frac{k-1}{n}\right)\right) & \frac{k-1}{n} \le s \le t \le \frac{k}{n} \\ U_n(t,r)U_n(r,s) & 0 \le s < r \le t \le 1 \end{cases}, \tag{1.16}$$

i.e. one splits the interval $[0,1]$ into n parts and replaces the generator on the small interval by a constant approximation. The nth approximation is then obtained by composing the short-time propagators. When one considers the limit $\lim_{n\to\infty} U_n$, it turns out that its existence is related to the operator

$$C(t,s) = A(t)A(s)^{-1} - \mathrm{id}.$$

One has

1.12 Theorem ([RS75], Theorem X.70)**.** *Let X be a Banach space and let I be an open interval in $\mathbb{R}$. For each $t \in I$, let $A(t)$ be the generators of a contraction semigroup on X so that 0 lies in the resolvent set $\rho(A(t))$ of $A(t)$ and assume that*

1. *the $A(t)$ have a common domain $\mathcal{D}$,*
2. *for each $\varphi \in X$, $(t-s)^{-1}C(t,s)\varphi$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact subinterval of I,*
3. *for each $\varphi \in X$, $C(t)\varphi := \lim_{s\to t}(t-s)^{-1}C(t,s)\varphi$ exists uniformly for t in each compact subinterval and $C(t)$ is bounded and strongly continuous in t.*

Then for all $s \leq t$ in any compact subinterval of I and for any $\varphi \in X$,

$$U(t,s)\varphi = \lim_{n\to\infty} U_n(t,s)\varphi$$

exists uniformly in s and t. Further, if $\psi \in \mathcal{D}$, then $\varphi_s(t) = U(t,s)\psi$ is in $\mathcal{D}$ for all t and satisfies

$$\frac{d}{dt}\varphi_s(t) = -A(t)\varphi_s(t), \qquad \varphi_s(s) = \psi$$

and $\|\varphi_s(t)\| \leq \|\psi\|$ for all $t \geq s$.

From this, we derive

1.13 Proposition. *Let $h^\varepsilon(t) = h_0(t) + \varepsilon h_1(t)$ be a time-dependent family of real subquadratic Hamiltonians. Then there is a unique unitary propagator associated to* (1.8)*.*

Proof. The proof uses the operators

$$A^{\pm}(t) := \pm i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))} + 1,$$

where $\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}$ denotes the closure of $\mathrm{op}^\varepsilon(h^\varepsilon(t))$. In the first step, we will establish that these operators are generators of contraction semigroups with $0 \in \rho(A^{\pm}(t))$. As $\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}$ is self-adjoint, we have $]-\infty, 1[\in \rho(A^{\pm}(t))$. Moreover,

$$\begin{aligned}\left\|[\lambda \pm i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))} + 1]\varphi\right\|^2 &= (\lambda+1)^2\|\varphi\|^2 + \left\|\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}\varphi\right\|^2 \\ &\quad \pm (\lambda+1)\left\langle i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}\varphi\middle|\varphi\right\rangle_{L^2(\mathbb{R}^d)} \pm (\lambda+1)\left\langle\varphi\middle|i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}\varphi\right\rangle_{L^2(\mathbb{R}^d)} \\ &= (\lambda+1)^2\|\varphi\|^2 + \left\|\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}\varphi\right\|^2 \geq \lambda^2\|\varphi\|^2\end{aligned}$$

for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $\lambda > 0$. Thus

$$\left\|[\lambda + (\pm i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))} + 1)]^{-1}\psi\right\| \leq \lambda^{-1}\|\psi\|$$

for all ψ in $A^+\mathcal{S}(\mathbb{R}^d)$ or $A^-\mathcal{S}(\mathbb{R}^d)$ respectively. As $-\lambda \in \rho(A^{\pm})$, these sets are dense in $L^2(\mathbb{R}^d)$ and the Hille-Yoshida Theorem (Theorem X.47a in [RS75]) shows that the $A^{\pm}(t)$ are generators of contraction semigroups.

For the other conditions, we use a Taylor expansion with respect to t to compute

$$\begin{aligned}\mathrm{op}^\varepsilon(h^\varepsilon(t))\varphi(x) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}h^\varepsilon\left(t,\frac{x+x'}{2},\xi\right)\varphi(x')\,dx'\,d\xi \qquad (1.17)\\ &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}h^\varepsilon\left(s,\frac{x+x'}{2},\xi\right)\varphi(x')\,dx'\,d\xi\\ &\quad+(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}\int_s^t\left(\frac{d}{dt}h^\varepsilon\right)\left(\tau,\frac{x+x'}{2},\xi\right)\,d\tau\varphi(x')\,dx'\,d\xi.\end{aligned}$$

Hence

$$\mathrm{op}^\varepsilon(h^\varepsilon(t))=\mathrm{op}^\varepsilon(h^\varepsilon(s))+\mathrm{op}^\varepsilon(g^\varepsilon)$$

where

$$g^\varepsilon(t,s,x,\xi)=\int_s^t\left(\frac{d}{dt}h^\varepsilon\right)(\tau,x,\xi)\;d\tau\in S[0;2d].$$

Now $\mathrm{op}^\varepsilon(g^\varepsilon)$ extends to a bounded linear operator on $L^2(\mathbb{R}^d)$. Thus by Theorem $X.13$ in [RS75], the domains of $\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}$ and $\overline{\mathrm{op}^\varepsilon(h^\varepsilon(s))}$ coincide and all $A^\pm$ have the same domain.

Moreover, by the assumptions on h_0 and h_1, the correspondence $(t,s)\to\mathrm{op}^\varepsilon(g^\varepsilon)$ is continuous in the uniform operator norm, which yields the continuity of $t\to(A^\pm(t))^{-1}$ with respect to t in the uniform operator norm, compare Theorem II-3.11. in [Kat66].

$C^\pm(t,s)$ is given by

$$C^\pm(t,s)=\mathrm{op}^\varepsilon(g^\varepsilon)(A^\pm(s))^{-1}$$

and hence uniform continuous with respect to (t,s). Finally we have the uniform limit

$$\lim_{s\to t}(t-s)^{-1}g^\varepsilon(t,s,x,\xi)=h_t^\varepsilon(t,x,\xi)$$

and hence

$$\lim_{s\to t}(t-s)^{-1}C^\pm(t,s)=\mathrm{op}^\varepsilon(h_t^\varepsilon)(A^\pm(t))^{-1},$$

which yields condition 3 of Theorem 1.12.

Having shown the existence of contraction semigroups $U^\pm(t,s)$ associated to $A^\pm(t)$, we set

$$\widetilde{U}(t,s)=\begin{cases}U^+(t,s) & s\le t\\ U^-(s,t) & t\le s\end{cases}$$

and

$$U(t,s):=e^{|t-s|}\widetilde{U}(t,s).$$

It remains to show that $U(t,s)$ is a unitary propagator and solves (1.8). If $t>s$, $U(t,s)$ is the limit of the operators $e^{t-s}U_n^+$. We consider one of the short-time propagators of (1.16) for some time t_0. One has

$$\frac{d}{dt}\exp\left(-(t-s)A^+(t_0)\right)\varphi=-A^+(t_0)\varphi=-i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t_0))}\varphi-\varphi$$

for all $\varphi\in\mathcal{D}(\mathrm{op}^\varepsilon(h^\varepsilon(t_0))$ and thus

$$\frac{d}{dt}\left[e^{t-s}\exp\left(-(t-s)A^+(t_0)\right)\right]\varphi=-i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t_0))}\left[e^{t-s}\exp\left(-(t-s)A^+(t_0)\right)\right]\varphi,$$

i.e. $e^{t-s}\exp\left(-(t-s)A^+(t_0)\right)$ is generated by $\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t_0))}$ and thus unitary, so $U(t,s)$ is unitary as the strong limit of unitary operators. In the same way, one shows that $U(t,s)$ fulfills

$$\frac{d}{dt}U(t,s)\varphi = -i\overline{\mathrm{op}^\varepsilon(h^\varepsilon(t))}U(t,s)\varphi$$

for all $\varphi \in \mathcal{D}(\overline{\mathrm{op}^\varepsilon(h^\varepsilon(s))})$ and $s > t$. It remains to show the composition formula

$$U(t,s) = U(t,r)U(r,s)$$

in the case where $U(t,r)$ and $U(r,s)$ arise from different generators. Let $s \le t \le r$. We have

$$\begin{aligned}
U(t,r)U(r,s) &= e^{|t-s|}U^-(r,t)e^{|r-s|}U^+(r,s) \\
&= \left[e^{|t-s|}U^+(t,s) + \int_t^r \frac{d}{d\tau}\left[e^{|\tau-t|}U^-(\tau,t)e^{|\tau-s|}U^+(\tau,s)\right]d\tau\right] \\
&= \left[e^{|t-s|}U^+(t,s) + \int_t^r \left[e^{|\tau-t|}U^-(\tau,t)[(1-A^-)+(1-A^+)]e^{|\tau-s|}U^+(\tau,s)\right]d\tau\right] \\
&= e^{|t-s|}U^+(t,s)
\end{aligned}$$

on $\mathcal{D}(\mathrm{op}^\varepsilon(h^\varepsilon(s)))$. A similar argument for the case $r \le s \le t$ concludes the proof of existence.

For the uniqueness, assume that U and $\widetilde{U}$ are two propagators of (1.8). We have

$$\begin{aligned}
U(t,s) - \widetilde{U}(t,s) &= -U(t,s)\int_s^t \frac{d}{d\tau}\left[U(s,\tau)\widetilde{U}(\tau,s)\right]d\tau \\
&= -U(t,s)\int_s^t \left[U(s,\tau)\left[\frac{i}{\varepsilon}\mathrm{op}^\varepsilon(h^\varepsilon(\tau)) - \frac{i}{\varepsilon}\mathrm{op}^\varepsilon(h^\varepsilon(\tau))\right]\widetilde{U}(\tau,s)\right]d\tau = 0
\end{aligned}$$

on the dense set $\mathcal{D}(\mathrm{op}^\varepsilon(h^\varepsilon(s)))$, where we used that a propagator fulfills

$$U(t,s)\mathcal{D}(\mathrm{op}^\varepsilon(h^\varepsilon(s))) \subset \mathcal{D}(\mathrm{op}^\varepsilon(h^\varepsilon(t)).$$

□

2 The classical system

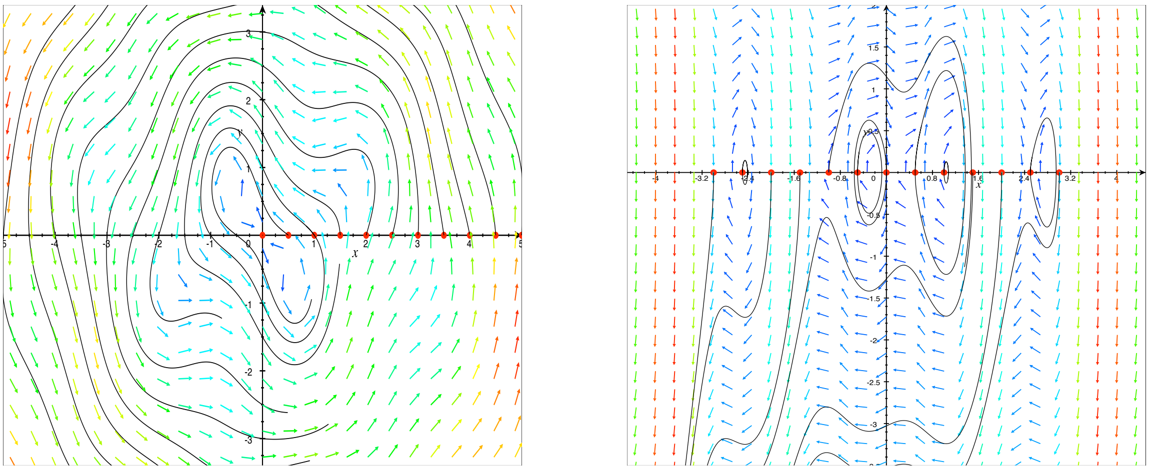

Figure 2.1: Classical flows associated to h_1 and h_2

We turn to the classical mechanics associated to the symbol. Our main focus lies on the growth properties of the classical flow with respect to the initial data. Figure 2.1 shows the flows associated to the Hamiltonians

$$h_1(x, \xi) = -\xi^2/2 - x^2/2 + \sin(2x)\cos(\xi) \quad \text{and}$$
$$h_2(x, \xi) = \xi^2/2 + x^3/3 + x\cos(3x).$$

In the first case one recognises an distorted rotation of the phase space. Trajectories, which have nearby starting points (indicated by the red dots) stay close to each other as time evolves. In the second case, the behavior of the Hamiltonian vector field is much more complicated. Depending on the initial position, the trajectories either follow a circular motion or they escape to infinity. Moreover, the behavior of a trajectory cannot be predicted from its neighbors, so the time-evolution “behaves badly” with respect to the initial phase space coordinates.

2.1 Canonical transformations of class $\mathcal{B}$

To introduce the notion of a canonical transformation, we recall that the symplectic group $\mathrm{Sp}(d)$ is the set of all matrices, which leave the symplectic form

$$v \wedge w = v \cdot Jw, \quad v, w \in \mathbb{R}^{2d}, \quad J := \begin{pmatrix} 0 & \mathrm{id} \\ -\mathrm{id} & 0 \end{pmatrix}$$

invariant, i.e.

$$\mathrm{Sp}(d) = \left\{ A \in \mathbb{R}^{2d \times 2d} \middle| A^\dagger J A = J \right\}.$$

It is well-known that $\mathrm{Sp}(d)$ is a subgroup of $\mathrm{Gl}(2d)$, where the inverse of a symplectic matrix A is given by $A^{-1} = -JA^\dagger J$.

2.1 Definition (Canonical transformation)**.**
A diffeomorphism $\kappa(q,p) = (X^\kappa(q,p), \Xi^\kappa(q,p)) \in C^\infty(\mathbb{R}^{2d}, \mathbb{R}^{2d})$ of $\mathbb{R}^{2d}$ is called a ***canonical transformation*** *if its Jacobian*

$$F^\kappa(q,p) = \begin{pmatrix} X_q^\kappa(q,p)^\dagger & X_p^\kappa(q,p)^\dagger \\ \Xi_q^\kappa(q,p)^\dagger & \Xi_p^\kappa(q,p)^\dagger \end{pmatrix}$$

is symplectic for all $(q,p) \in \mathbb{R}^{2d}$.

In the appendix, we collect some relations between the block-matrices from which $F^\kappa(q,p)$ is build. The following definition makes the class of canonical transformations with a "controlled dependence" on the initial data more precise. The definition is inspired by the one in [Fuj79], where a related notion for smooth diffeomorphism from $\mathbb{R}^d$ to $\mathbb{R}^d$ is introduced.

2.2 Definition (Class $\mathcal{B}$)**.** *A time-dependent family of canonical transformations $\kappa^t, t \in]-T,T[$, $T \in \mathbb{R} \cup \{+\infty\}$ is* ***of class*** $\mathcal{B}$ *if it is pointwise continuously differentiable with respect to time and we have*

$$\sup_{t \in]-T,T[} \left\| \partial^\alpha_{(q,p)} F^{\kappa^t}(q,p) \right\| < \infty \quad \text{and} \quad \sup_{t \in]-T,T[} \left\| \partial^\alpha_{(q,p)} \frac{d}{dt} F^{\kappa^t}(q,p) \right\| < \infty$$

for all $|\alpha| \geq 0$. The definition extends in a natural way to a time-independent canonical transformation.

The property, which makes canonical transformations of class $\mathcal{B}$ so interesting is that they are Lipschitz-continuous with respect to the phase-space variables, i.e. one has good control on the dependence of $\kappa(q,p)$ with respect to (q,p). Moreover, the inverse transformation is in the same class.

2.3 Proposition.

1. *The canonical transformations of class $\mathcal{B}$ are a subgroup of the diffeomorphisms of $\mathbb{R}^{2d}$.*
2. *If κ is a canonical transformation of class $\mathcal{B}$, there exist $c_\kappa, C_\kappa > 0$ such that*

$$c_\kappa \|(q_1,p_1) - (q_2,p_2)\| \leq \|\kappa(q_1,p_1) - \kappa(q_2,p_2)\| \leq C_\kappa \|(q_1,p_1) - (q_2,p_2)\| \tag{2.1}$$

for all $(q_1,p_1),(q_2,p_2) \in \mathbb{R}^{2d}$.

Proof.

1. We show that the inverse and the composition of canonical transformations of class $\mathcal{B}$ are canonical transformations of class $\mathcal{B}$. For canonical transformations κ and κ' of class $\mathcal{B}$, we have

$$F^{\kappa\circ\kappa'} = (F^\kappa \circ \kappa') F^{\kappa'}$$

by the chain rule. Moreover, by the Leibniz-rule $M_k^{\kappa\circ\kappa'} := M_k^0 \left[F^{\kappa'\circ\kappa} \right]$ (defined in (1.7)) is bounded by a polynomial in M_l^κ and $M_{l'}^{\kappa'}$ for $l, l' \leq k$.

Setting $\kappa' = \kappa^{-1}$, we have

$$F^{\kappa^{-1}} = (F^\kappa \circ \kappa^{-1})^{-1} = -J(F^\kappa \circ \kappa^{-1})^\dagger J.$$

Hence $M_0^{\kappa^{-1}}$ is bounded by M_0^κ. Moreover we see that derivatives of order k of $F^{\kappa^{-1}}$ (i.e. derivatives of order $k+1$ of κ^{-1}) depend on derivatives of order k of F^κ and κ^{-1}. Thus we see inductively that $M_k^{\kappa^{-1}}$ is bounded by a polynomial in M_l^κ for $l \leq k$.

2. By the mean value inequality, we have

$$\|\kappa(q_1,p_1) - \kappa(q_2,p_2)\| \leq \sup_{(q,p)\in\mathbb{R}^{2d}} \|F^\kappa(q,p)\| \, \|(q_1,p_1) - (q_2,p_2)\|$$

and

$$\begin{aligned}\|(q_1,p_1) - (q_2,p_2)\| &= \left\|(\kappa^{-1}\circ\kappa)(q_1,p_1) - (\kappa^{-1}\circ\kappa)(q_2,p_2)\right\| \\ &\leq \sup_{(q,p)\in\mathbb{R}^{2d}} \left\|F^{\kappa^{-1}}(q,p)\right\| \|\kappa(q_1,p_1) - \kappa(q_2,p_2)\| .\end{aligned}$$

Thus (2.1) holds with $C_\kappa = M_0^\kappa$ and $c_\kappa = [M_0^{\kappa^{-1}}]^{-1}$.

□

2.2 Actions associated to canonical transformations

A central quantity related to canonical transformations is the action. Actually, the classical mechanics can be derived from the principle of stationary action. Depending on context and purpose, the action shows up in many formulations. As starting point of classical mechanics it is often considered as a functional of trajectories, but already given a canonical transformation, it can be useful to consider it as a function of q and $X^\kappa(q,p)$, compare [Fuj79]. We use the following formulation:

2.4 Definition (Action). *Let $\kappa = (X^\kappa(q,p), \Xi^\kappa(q,p))$ be a canonical transformation of $\mathbb{R}^{2d}$. A real-valued function S^κ is called an* ***action associated to*** *κ if it fulfills*

$$S_q^\kappa(q,p) = -p + X_q^\kappa(q,p)\Xi^\kappa(q,p) \qquad \text{and} \qquad S_p^\kappa(q,p) = X_p^\kappa(q,p)\Xi^\kappa(q,p)$$

for all $(q,p) \in \mathbb{R}^{2d}$. For a time-dependent family of canonical transformations κ^t, we call a function $S^{\kappa^t} \in C^\infty(\mathbb{R}^{2d+1}, \mathbb{R})$ an action associated to κ^t, if S^{κ^t} an action associated to κ^t pointwise in time.

We collect some properties of S^κ. In particular, we will show that for the case of a time-dependent family of canonical transformations, the action can be chosen smooth with respect to time.

2.5 Proposition.

1. *For every canonical transformation of $\mathbb{R}^{2d}$ there is an action associated to it.*

2. *An action is unique up to an additive constant.*

3. *If κ and κ' are canonical transformations, then $S^{\kappa'} \circ \kappa + S^{\kappa}$ is an action associated to $\kappa' \circ \kappa$. In particular $-S^{\kappa} \circ \kappa^{-1}$ is an action associated to κ^{-1}.*

4. *If κ^t is a family of canonical transformations of class $\mathcal{B}$, the time-dependent constant can be chosen such that $S^{\kappa^t} \in C^\infty(]-T,T[\times\mathbb{R}^{2d})$ with $S_t(t,q,p) \in S[2;2d]$ for all $t \in]-T,T[$.*

Proof.

1. If S^κ is an action associated to κ, we have

$$\begin{aligned}\frac{d}{d\tau}S^\kappa(\tau q,\tau p) &= S^\kappa_q(\tau q,\tau p)\cdot q + S^\kappa_p(\tau q,\tau p)\cdot p\\ &= -\tau p\cdot q + X^\kappa_q(\tau q,\tau p)\Xi^\kappa(\tau q,\tau p)\cdot q + X^\kappa_p(\tau q,\tau p)\Xi^\kappa(\tau q,\tau p)\cdot p\\ &= -\tau p\cdot q + \Xi^\kappa(\tau q,\tau p)\cdot\frac{d}{d\tau}X^\kappa(\tau q,\tau p).\end{aligned}$$

This motivates the definition of the function

$$S^\kappa(q,p) := \int_0^1 \left(-\tau p\cdot q + \Xi^\kappa(\tau q,\tau p)\cdot\frac{d}{d\tau}X^\kappa(\tau q,\tau p)\right)\, d\tau \tag{2.2}$$

which actually is an action associated to κ. Indeed

$$\begin{aligned}&S^\kappa_q(q,p)\\ &= \int_0^1\left\{-\tau p + \tau\Xi^\kappa_q(\tau q,\tau p)\left[\frac{d}{d\tau}X^\kappa(\tau q,\tau p)\right] + \left[\frac{d}{d\tau}\tau X^\kappa_q(\tau q,\tau p)\right]\Xi^\kappa(\tau q,\tau p)\right\}\, d\tau\\ &= \int_0^1\left\{-2\tau p + \left[X^\kappa_q(q,p)\Xi^\kappa_p(q,p)^\dagger - \Xi^\kappa_q(q,p)X^\kappa_p(q,p)^\dagger\right]p\right.\\ &\quad+\quad \tau\left[\Xi^\kappa_q(\tau q,\tau p)X^\kappa_q(\tau q,\tau p)^\dagger q + \Xi^\kappa_q(\tau q,\tau p)X^\kappa_p(\tau q,\tau p)^\dagger p\right]\\ &\quad+\quad \left.\left[\frac{d}{d\tau}\tau X^\kappa_q(\tau q,\tau p)\right]\Xi^\kappa(\tau q,\tau p)\right\}\, d\tau\\ &= \int_0^1\left\{\frac{d}{d\tau}\left[-\tau^2 p + \tau X^\kappa_q(\tau q,\tau p)\Xi^\kappa(\tau q,\tau p)\right]\right\}\, d\tau = -p + X^\kappa_q(q,p)\Xi^\kappa(q,p),\end{aligned}$$

where we used the symplecticity of $F^\kappa(q,p)$. The identity $S^\kappa_q(q,p) = X^\kappa_q(q,p)\Xi^\kappa(q,p)$ follows from a similar computation.

2. Let S^κ_1 and S^κ_2 be two actions associated to κ. The uniqueness up to additive constants follows from

$$\begin{aligned}S^\kappa_1(q,p) - S^\kappa_2(q,p) &= S^\kappa_1(0,0) - S^\kappa_2(0,0) + \int_0^t \frac{d}{d\tau}\left[S^\kappa_1(\tau q,\tau p) - S^\kappa_2(\tau q,\tau p)\right]\, d\tau\\ &= S^\kappa_1(0,0) - S^\kappa_2(0,0).\end{aligned}$$

3. We have

$$\begin{aligned}
\left(S^{\kappa'}\circ\kappa+S^{\kappa}\right)_q &= X_q^{\kappa}(q,p)\left(S_q^{\kappa'}\circ\kappa\right)(q,p)+\Xi_q^{\kappa}(q,p)\left(S_p^{\kappa'}\circ\kappa\right)(q,p)+S_q^{\kappa}(q,p)\\
&= X_q^{\kappa}(q,p)\left(-\Xi^{\kappa}(q,p)+\left(X_q^{\kappa'}\circ\kappa\right)(q,p)\Xi^{\kappa'\circ\kappa}(q,p)\right)\\
&\quad+\Xi_q^{\kappa}(q,p)\left(X_p^{\kappa'}\circ\kappa\right)(q,p)\Xi^{\kappa'\circ\kappa}(q,p)-p+X_q^{\kappa}(q,p)\Xi^{\kappa}(q,p)\\
&= -p+X_q^{\kappa}(q,p)\left(X_q^{\kappa'}\circ\kappa\right)(q,p)\Xi^{\kappa'\circ\kappa}(q,p)\\
&\quad+\Xi_q^{\kappa}(q,p)\left(X_p^{\kappa'}\circ\kappa\right)(q,p)\Xi^{\kappa'\circ\kappa}(q,p)\\
&= -p+X_q^{\kappa'\circ\kappa}(q,p)\Xi^{\kappa'\circ\kappa}(q,p)
\end{aligned}$$

and

$$\left(S^{\kappa'}\circ\kappa+S^{\kappa}\right)_p = X_p^{\kappa'\circ\kappa}(q,p)\Xi^{\kappa'\circ\kappa}(q,p)$$

by a completely analogous computation.

4. The explicit action defined in (2.2) fulfills the assertions.

□

2.3 Hamiltonian flows

We are particularly interested in Hamiltonian flows associated to the symbols of our Hamiltonians, i.e. time-dependent families of canonical transformations $\kappa^{(t,s)}$, which obey Hamilton's equation of motion

$$\frac{d}{dt}\kappa^{(t,s)} = J\nabla_{(x,\xi)}h\left(t,\kappa^{(t,s)}\right),\quad \kappa^{(s,s)}=\mathrm{id}. \tag{2.3}$$

We recall a well-known relation between quadratic Hamiltonians and linear flows:

2.6 Proposition. *An Hamiltonian flow is linear if and only if it is generated by a quadratic Hamiltonian.*

Proof. Differentiating (2.3) with respect to (q,p) yields

$$\frac{d}{dt}F^{\kappa^{(t,s)}}(q,p) = J\mathrm{Hess}_{(x,\xi)}h\left(t,\kappa^{(t,s)}(q,p)\right)F^{\kappa^{(t,s)}}(q,p). \tag{2.4}$$

If h is quadratic, the Hessian does not depend on q and p, i.e.

$$\mathrm{Hess}_{(x,\xi)}h\left(t,\kappa^{(t,s)}(q,p)\right)=M(t)$$

and it follows from ODE-theory that the solution of (2.4) is linear in (q,p), see Corollary 2 in Section 27 of [Arn73].

Now consider a linear Hamiltonian flow, i.e. $\kappa^{(t,s)}(q,p)=M(t,s)(q,p)$. We set

$$h(t,q,p) := \begin{pmatrix} q & p\end{pmatrix} J\left(\frac{d}{dt}M(t,s)\right)JM(t,s)^{\dagger}J\begin{pmatrix} q\\ p\end{pmatrix}$$

and claim that $h(t,q,p)$ generates $\kappa^{(t,s)}$. It is easily checked that the so-defined Hamiltonian fulfills (2.4). Thus $\kappa^{(t,s)}$ coincides with the flow generated by h by the Picard-Lindelöff-Theorem.

□

More generally speaking, we have a correspondence between canonical transformations of class $\mathcal{B}$ and subquadratic Hamiltonians, i.e. the symbols we already met in the context of essential self-adjointness:

2.7 Proposition. *If $h \in C^\infty(\mathbb{R}^{2d+1}, \mathbb{R})$ is a time-dependent subquadratic Hamiltonian, the Hamiltonian flow $\kappa^{(t,s)}$ generated by h is a family of canonical transformations of class $\mathcal{B}$ in $[-T, T]$. Conversely, every Hamiltonian flow of class $\mathcal{B}$ is generated by a subquadratic Hamiltonian.*

Moreover, if

$$K_k^h = \max_{|\alpha|=k} \sup_{(t,x,\xi)\in\mathbb{R}^{2d+1}} \left\| \partial^\alpha_{(x,\xi)} \mathrm{Hess}_{(x,\xi)} h(t,x,\xi) \right\| < \infty$$

for all $k \leq n_0$, we have

$$\sup_{|t-s|<T(\varepsilon)} M_k^0 \left[F^{\kappa^{(t,s)}} \right] \leq C_k (2C_T)^k \left|\log \varepsilon\right|^k \varepsilon^{-2K[h]C_T}, \tag{2.5}$$

for all $k \leq n_0$ on the Ehrenfest timescale $T(\varepsilon) = C_T \log \varepsilon^{-1}$, where

$$K[h] = \sup_{(t,q,p)\in\mathbb{R}^{2d+1}} \sup_{\substack{X\in\mathbb{R}^{2d} \\ \|X\|=1}} \left| \left\langle \mathrm{JHess}_{(x,\xi)} h(t,x,\xi) X, X \right\rangle \right| .$$

For convenience of the reader, we quote the main tool of the proof.

2.8 Lemma (Gronwall)**.** *Let $f, \alpha \in C([a,b], \mathbb{R})$, $\beta \in C([a,b], [0, +\infty[)$ for some compact interval $[a,b] \subset \mathbb{R}$. If*

$$f(t) \leq \alpha(t) + \int_a^t \beta(\tau) f(\tau)\, d\tau$$

for all $t \in [a,b]$, we have

$$f(t) \leq \alpha(t) + \int_a^t \alpha(\tau)\beta(\tau) e^{\int_\tau^t \beta(\sigma)\, d\sigma}\, d\tau$$

for all $t \in [a,b]$.

Proof. By (2.4) and the fundamental theorem of calculus, we have

$$\begin{aligned} \left| F^{\kappa^{(t,s)}} X \right|^2 &= 2 \int_s^t \left\langle \mathrm{JHess}_{(x,\xi)} h \left(\tau, \kappa^{(\tau,s)}(q,p) \right) F^{\kappa^{(\tau,s)}}(q,p) X \middle| F^{\kappa^{(\tau,s)}}(q,p) X \right\rangle \, d\tau + |X|^2 \\ &\leq 2K[h](T) \left| \int_s^t \left| F^{\kappa^{(\tau,s)}}(q,p) X \right|^2 \, d\tau \right| + |X|^2 \end{aligned}$$

for all $X \in \mathbb{R}^{2d}$, where

$$K[h](T) = \sup_{t\in]-T,T[} \sup_{(q,p)\in\mathbb{R}^{2d}} \sup_{\substack{X\in\mathbb{R}^{2d} \\ \|X\|=1}} \left| \left\langle \mathrm{JHess}_{(x,\xi)} h(t,x,\xi) X, X \right\rangle \right| .$$

We deduce

$$\left\| F^{\kappa^{(t,s)}}(q,p) \right\| \leq e^{K[h](T)|t-s|}$$

by an application of Gronwall's Lemma.

The estimate

$$\left\|\partial^{\alpha}_{(q,p)} F^{\kappa^{(t,s)}}(q,p)\right\| \le C_k (2T)^k e^{K[h](T)|t-s|},$$

is proved inductively. We have

$$\begin{aligned}
\left\|\partial^{\alpha}_{(q,p)} F^{\kappa^{(t,s)}}(q,p)\right\| &\le \left|\int_s^t K[h](T)\left\|\partial^{\alpha}_{(q,p)} F^{\kappa^{(\tau,s)}}(q,p)\right\| \, d\tau\right| \\
&\quad + \left|\int_s^t \sum_{\beta<\alpha}\binom{\alpha}{\beta}\left\|\partial^{\alpha-\beta}_{(q,p)}\left[\mathrm{Hess}_{(x,\xi)} h(\tau,\kappa^{(\tau,s)}(q,p))\right]\partial^{\beta}_{(q,p)} F^{\kappa^{(t,s)}}(q,p)\right\| \, d\tau\right| \\
&\le \left|\int_s^t K[h](T)\left\|\partial^{\alpha}_{(q,p)} F^{\kappa^{(\tau,s)}}(q,p)\right\| \, d\tau\right| \\
&\quad + \left|\int_s^t \sum_{\beta<\alpha}\binom{\alpha}{\beta} K^h_{|\alpha-\beta|}(T) C_{|\beta|}(2T)^{|\beta|} e^{K[h](T)|\tau-s|} \, d\tau\right|.
\end{aligned}$$

Setting (and assuming $T > 1$)

$$C'_k := \sum_{\beta<\alpha}\binom{\alpha}{\beta} K^h_{|\alpha-\beta|}(T) C_{|\beta|},$$

Gronwall's Lemma provides

$$\begin{aligned}
&\left\|\partial^{\alpha}_{(q,p)} F^{\kappa^{(t,s)}}(q,p)\right\| \\
&\le \left|\int_s^t C'_k (2T)^{|\alpha|-1} e^{K[h](T)|\tau-s|} \, d\tau\right| \\
&\quad + \left|\int_s^t \left[\int_s^\tau C'_k (2T)^{|\alpha|-1} e^{K[h](T)|\sigma-s|} \, d\sigma\right] K[h](T) e^{\left|\int_\tau^t K[h](T)\, d\sigma\right|}\right| \\
&\le C'_k (2T)^{|\alpha|} e^{K[h](T)|t-s|} + \left|\int_s^t C'_k (2T)^{|\alpha|-1} e^{K[h](T)|\tau-s|} K[h](T) e^{K[h](T)|t-\tau|} \, d\tau\right| \\
&\le C'_k (1 + K[h](T))(2T)^{|\alpha|} e^{K[h](T)|t-s|}.
\end{aligned}$$

The result for the Ehrenfest timescale follows by substituting $T(\varepsilon) = C_T \log(\varepsilon^{-1})$ into this expression.

Now consider a Hamiltonian flow of class $\mathcal{B}$ generated by some Hamilton function h. The identity (2.4) gives

$$J\left(\frac{d}{dt} F^{\kappa^{(t,s)}}(q,p)\right) J\left(F^{\kappa^{(t,s)}}(q,p)\right)^{\dagger} J = \mathrm{Hess}_{(q,p)} h(t,\kappa^{(t,s)}(q,p)).$$

Hence, h is subquadratic, as $\left(\frac{d}{dt} F^{\kappa^{(t,s)}}\right)$ is of class $S[0; 2d]$ by definition. □

2.4 The Ehrenfest-timescale

We close this part with a discussion of the timescale $T(\varepsilon) = C_T \log \varepsilon^{-1}$, for which we established (2.5). This Ehrenfest timescale is the longest timescale, on which semiclassical approximations can in general hold. However, for special cases in special cases, semiclassical approximations may hold much longer. A prominent example is the harmonic oscillator, for which semiclassical approximations are exact for all times.

Estimate (2.5) is at the basis of the proofs of all results on the Ehrenfest timescale. Among them are [HJ00] and [CR97], where it is shown that expressions like (0.6) for the approximate time-evolution of coherent states hold on the Ehrenfest timescale. Other relevant works are [DBR03], where the time-evolution of expectation values with respect to certain localised states is studied and the papers [BGP99] and [BR02], which investigate the propagation of observables with error bounds in operator norm. Finally, [BB79] studies the time-evolution of the Wigner function.

The core of all these papers it that the error of semiclassical approximations depends on derivatives of the classical flow. Now (2.5) shows that these derivatives grow polynomially in $\log\left(\varepsilon^{-1}\right)$. Thus they can be controlled, if one has established an $O(\varepsilon)$ error estimate. If on the other hand the growth of the timescale is faster than $C_T \log \varepsilon^{-1}$, the derivatives will in general explode exponentially in ε^{-1}.

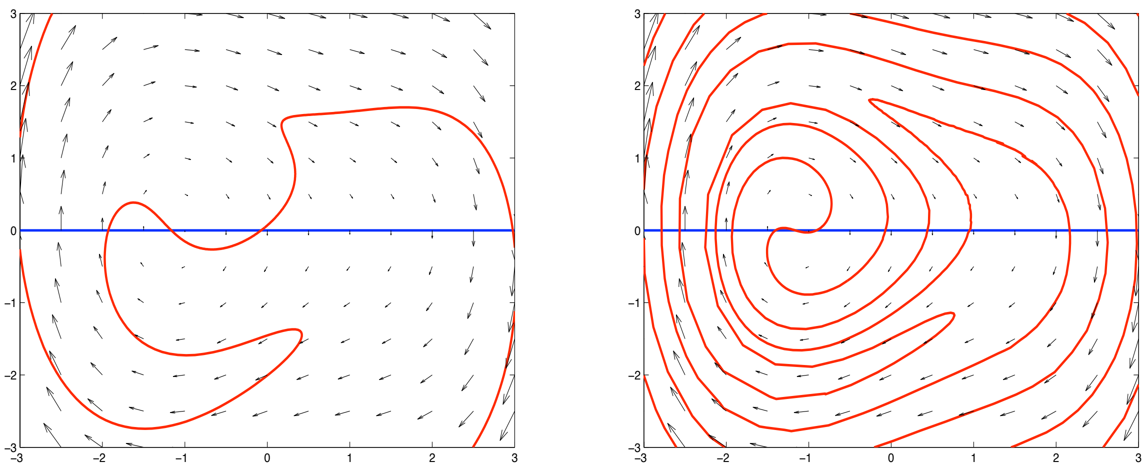

Figure 2.2: $\Phi^{\kappa^t}(\mathcal{L}_S)$ for $\mathcal{L}_S = \{(x,0)\}$ and the flow κ^t generated by $h(x,\xi) = \xi^2/2 + x^4 + \cos(x)$ for $t = 5$ and 25.

However, a more geometric interpretation is possible. The basis for this is the theory of Maslov [MF81], which we will discuss in detail in the next section, see also [Lit92] for an easily accessible review. The basic observation is that an WKB-type initial datum

$$\psi_0(x) = u(x) e^{\frac{i}{\varepsilon} S(x)}, \qquad u \in C_0^\infty(\mathbb{R}^d, \mathbb{C}), \quad S \in C^\infty(\mathbb{R}^d, \mathbb{R})$$

defines a Lagrangian manifold $\mathcal{L}_S$ in the phase-space $T^*(\mathbb{R}^d)$, which is given by

$$\mathcal{L}_S := \{(x, \nabla_x S(x))\} \subset T^*(\mathbb{R}^d).$$

This manifold is then transported along the classical flow $\kappa^{(t,s)}$ and the WKB-approximation

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

is reconstructed from $\kappa^{(t,s)}(\mathcal{L}_S)$. In [BBT79] Berry et al. investigate the structure of this manifold and observe that it develops "whorls" and "tendrils" when time progresses. When the Ehrenfest time is reached, these structures are only order ε apart. With respect to the WKB-approximation this means that $S(t,x)$ varies on a scale of ε such that the error term of the approximation is of order $O(1)$.

Part II

Fourier Integral Operators

3 Some remarks on global FIO theory

Before we introduce our operators, we discuss some aspects of global Fourier Integral Operators. In the first section we sketch the Hörmander-Maslov theory of global FIOs and elucidate the caustic problem, which is inherent to FIOs with real phase. As this traditional FIO theory is usually used in the context of distributions on manifolds, we will not state rigorous results here but focus on the principal ideas. At the end of this section, we will give a first survey on L^2-boundedness results on FIOs, where we will be more precise.

3.1 Hörmander-Maslov theory and the caustic problem

We turn back to the WKB-initial datum

$$\psi_0(x) = u(x)e^{\frac{i}{\varepsilon}S(x)}, \qquad u \in C_0^\infty(\mathbb{R}^d, \mathbb{C}), \quad S \in C^\infty(\mathbb{R}^d, \mathbb{R})$$

and the Lagrangian manifold

$$\mathcal{L}_S := \{(x, \nabla_x S(x))\} \subset T^*(\mathbb{R}^d).$$

In the WKB-approach one tries to approximate the solution of the time-dependent Schrödinger equation (1.8) by a wavepacket of the form

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

It is well known that this yields the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t}(t,x) - h\left(t,x,\nabla_x S\right) = 0, \quad S(s,x) = S(x) \tag{3.1}$$

for the action $S(t,x)$ and the transport equation

$$\frac{\partial}{\partial t}n(t,x) + \operatorname{div}\left[n(t,x)\partial_\xi h\left(t,x,\nabla_x S\right)\right], \quad n(s,x) = u^2(x), \tag{3.2}$$

for the amplitude, see e.g. [SMM03]. Here $u(t,x) = \sqrt{n(t,x)}$ and the square-root is chosen by continuity in time.

Maslov canonical operator

The Maslov-theory (see [Mas72] and [MF81]) allows for a geometric interpretation of the WKB method. Using the bicharacteristics

$$t \mapsto (q(t), p(t)) = \left(q(t), \nabla_x S(t,x)\right),$$

one obtains the following picture of the WKB-approximation (compare Figure 3.1).

1. The initial datum is associated with a function $\varphi_0 \in C_0^\infty(\mathcal{L}_S)$ by
$$\varphi_0(y, \nabla S(y)) := u(y).$$
2. The manifold $\mathcal{L}_S$ is transported along the Hamiltonian flow $\kappa^{(t,s)}$ associated to $h(t)$. This yields the manifold $\kappa^{(t,s)}(\mathcal{L}_S)$ and the function $\varphi^{\kappa^{(t,s)}} \in C_0^\infty\left(\kappa^{(t,s)}\left(\mathcal{L}_S\right)\right)$, which is defined as
$$\varphi^{\kappa^{(t,s)}}(q,p) = \varphi_0(\kappa^{-1}(q,p)) \qquad (q,p) \in \kappa^{(t,s)}\left(\mathcal{L}_S\right).$$
3. The function $u(t,s)$ is derived from the projection of $\varphi^{\kappa^{(t,s)}}$ onto $\mathbb{R}^d$.

Assuming that the mapping
$$y \mapsto X^{\kappa^{(t,s)}}(y, \nabla S(y))$$
is a diffeomorphism of $\mathbb{R}^d$, the solution is explicitly computable and reads
$$\psi_{\mathrm{WKB}}(t, X^{\kappa^{(t,s)}}(y, \nabla S(y))) = u_0(y)\sqrt{\frac{J(s,y)}{J(t,y)}}e^{\int_s^t \frac{1}{2}\mathrm{tr}\left(\partial_x\partial_\xi h\right)\circ\kappa^{(\tau,s)}(y,\nabla_x S(y))\,d\tau}, \tag{3.3}$$
where the quantity
$$J(t,y) = \det\left(\frac{\partial X^{\kappa^{(t,s)}}(y, \nabla S(y))}{\partial y}\right) \tag{3.4}$$
is related to the deformation of the manifold. Obviously, the solution breaks down if $J(t,x) = 0$ for some (t,x). In geometric terms this condition means that the tangent on the manifold $\kappa\left(\mathcal{L}_S\right)$ is parallel to the momentum axis such that the projections to $\mathbb{R}^d$ are not diffeomorphic any more, compare Figure 3.1. The nomenclature for such phenomena is derived from geometric optics. A WKB treatment of the Helmholtz-equation reveals the breakdown just described coincides with the situation that infinitely many light rays converge in the *focal point* y. Therefore, one calls the set of such points a *caustic*.

The principal idea of Maslov to overcome the caustic problem uses that a Lagrangian manifold locally always allows for diffeomorphic projections on a set of position and momentum coordinates. More precisely, for every point $(q,p) \in \kappa^{(t,s)}\left(\mathcal{L}_S\right)$, there is a basis $(f_1, \ldots, f_d)$, $f_j \in \{e_j, e_{d+j}\}$ of a d-dimensional subspace $X \subset \mathbb{R}^{2d}$ of the phase-space and a compact set $K \subset \mathbb{R}^{2d}$ containing a neighborhood of (q,p) such that the projection
$$\pi : K \cap \kappa\left(\mathcal{L}_S\right) \to X$$
of the manifold on X is a diffeomorphism. Moreover, there is a function $\widetilde{S}$ such that the manifold may locally be represented as
$$K \cap \kappa\left(\mathcal{L}_S\right) = \left\{(z, \nabla\widetilde{S}(z))\middle| z \in \pi(K)\right\}.$$
Assuming for simplicity that one has a pure momentum representation, one shows that the solution can be expressed with help the inverse Fourier-transform
$$u(t,x) = \left[\left(\mathcal{F}^\varepsilon\right)^{-1}\pi(\varphi^\kappa)(\cdot)e^{i\widetilde{S}(\cdot)/\varepsilon - i\pi\nu/2}\right](x), \tag{3.5}$$
where an additional phase is introduced by the *Morse index* $\nu \in \{0,1,2,3\}$.

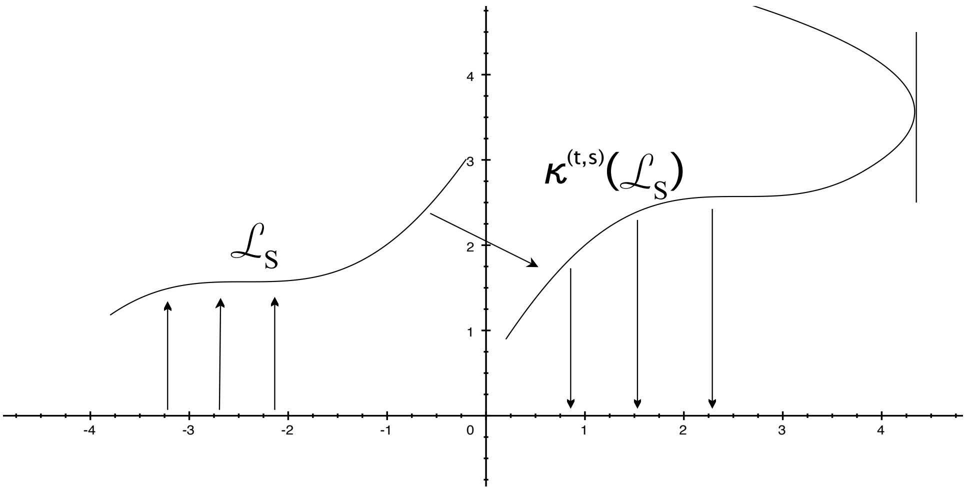

Figure 3.1: Geometric interpretation of WKB-method. Shown are the Lagrangian manifolds $\mathcal{L}_S$ and $\kappa^{(t,s)}(\mathcal{L}_S)$ in phase-space. The arrows illustrate the definition of the function φ and the projection of $\varphi^{\kappa^{(t,s)}}$ onto $\mathbb{R}^d$. The vertical tangent indicates a focal point.

Now the *Maslov canonical operator*

$$K : C_0^\infty(\kappa(\mathcal{L}_S)) \to C^\infty(\mathbb{R}^d)$$

is obtained from the globalization of this idea: exploiting the local existence of diffeomorphisms, one creates an atlas of the Lagrangian manifold $\kappa^{(t,s)}(\mathcal{L}_S)$, projects on the local coordinates and applies partial Fourier transforms to obtain a position representation. One can show that the obtained function is smooth for a proper choice of the Maslov indices and that the operator is invariant with respect to the choice of the atlas to order $O(\varepsilon)$ in L^2-norm, compare [MF81].

Global Fourier Integral Operators

The same geometric ideas are followed in the seminal works [Hör71] and [DH72] on global Fourier Integral Operators. This class of operators arises if one studies the solution of hyperbolic partial differential equations (see e.g. the introduction in [Tre80]). Formally they are given by

$$[\mathcal{I}^\varepsilon(\Phi, u)\varphi](x) = (2\pi\varepsilon)^{-(d+D)/2} \int_{\mathbb{R}^d}\int_{\mathbb{R}^D} e^{\frac{i}{\varepsilon}\Phi(x,y,\theta)} u(x,y,\theta)\varphi(y)\, d\theta\, dy, \tag{3.6}$$

where the real valued phase function $\Phi \in C^\infty(\mathbb{R}^{2d+D}, \mathbb{R})$ is homogeneous with respect to the covariable $\theta \in \mathbb{R}^D$. In particular, pseudodifferential operators are FIOs with phase function $\Phi(x, y, \theta) = \theta \cdot (x - y)$ and $D = d$.

As in the case of PDOs, one is confronted with the convergence of the integral for symbols which do not provide decay. If one tries to circumvent this problem with help of the smoothing approach of Lemma 1.3 or integration by parts as in Definition 1.2 it turns out that one has to assume the invertibility of the matrix

$$D(\Phi)(x, y, \theta) = \begin{pmatrix} \partial_{xy}\Phi & \partial_{x\theta}\Phi \\ \partial_{y\theta}\Phi & \partial_{\theta\theta}\Phi \end{pmatrix} \tag{3.7}$$

on the set

$$\Sigma_\Phi := \{(x, y, \theta) | \nabla_\theta \Phi(x, y, \theta) = 0\}. \tag{3.8}$$

The importance of the set (3.8) should not come as a surprise to the reader, which is familiar with asymptotic analysis, as the non-stationary phase argument shows that the integral in (3.6) is formally $O(\varepsilon^\infty)$ outside Σ_Φ.

For a geometric interpretation, one supposes that the differentials of $\partial_{\theta_j}\Phi$ with respect to x, y and θ are linearly independent on Σ_Φ, which assures that Σ_Φ is a manifold of maximal codimension in $\mathbb{R}^{2d+D}$. Moreover, the condition on the determinant (3.7) yields that the maps

$$\begin{aligned} \hat{\xi}: \quad & \Sigma_\Phi \to \mathbb{R}^{2d} \\ & (x,y,\theta) \mapsto \hat{\xi}(x,y,\theta) := (x, \xi(x,y,\theta)) := (x, \nabla_x \Phi(x,y,\theta)) \end{aligned}$$

$$\begin{aligned} \hat{\eta}: \quad & \Sigma_\Phi \to \mathbb{R}^{2d} \\ & (x,y,\theta) \mapsto \hat{\eta}(x,y,\theta) := (y, -\eta(x,y,\theta)) := (y, \nabla_y \Phi(x,y,\theta)) \end{aligned}$$

are diffeomorphisms. The connection with the Maslov theory in the case $D = d$ is the following: if one thinks of η as an initial momentum and of ξ as a final momentum, this diffeomorphism property is exactly the one which avoids the caustics.

There is even more connection between the two theories. The fundamental set of the global FIO theory

$$\mathcal{L}_\Phi = \{(x,y,\xi,\eta) \mid \exists\theta \text{ such that } \eta = \eta(x,y,\theta), \xi = \xi(x,y,\theta)\}$$

corresponds exactly to the graph $\mathcal{L}_S \times \kappa\,(\mathcal{L}_S)$ in the case of the Maslov theory. Now the extension of (3.6) beyond points, where (3.7) does not hold, follows the same geometric approach, i.e. one takes the viewpoint that a globally defined smooth Lagrangian manifold is the fundamental object to which the operator is associated and considers (3.6) as a local representation in special coordinates. The global operator then allows for a representation as a sum of operators of the form (3.6) or partial Fourier-transformations of such expressions.

FIOs with complex phase

The generalisation to FIOs with complex phase is due to Melin and Sjostrand [MS75]. In this theory, the Lagrangian manifold is replaced by a so-called almost Lagrangian manifold, which is, quoting [Tre80], "neither Lagrangian nor a manifold". The main advantage of this generalisation is that one can always find one global oscillatory integral representation for a Fourier Integral Operator, which is associated to a canonical transformation, see [LSV94]. The operators we will define are a special class of such FIOs. Because of the global representation as an oscillatory integral, we will not need the geometric background for their treatment, but the connection to geometric objects, more precisely to the graph of a canonical transformation shines through nevertheless. This applies especially to Definition 4.4 and Proposition 4.13.

3.2 On the L^2-continuity of FIOs

Though FIOs are primarily aimed at hyperbolic PDEs and are thus usually treated in the distributional setting, there are several results on L^2-boundedness properties of FIOs with real phase. First of all, the standard result that FIOs are bounded from $L^2_{\mathrm{loc}}(\mathbb{R}^d)$ and $L^2_{\mathrm{c}}(\mathbb{R}^d)$ into themselves respectively appears already in [Hör71].

The first global L^2-boundedness result on FIOs with real phase is due Kumano-Go [KG76]. In the case $D = d$ and $\varepsilon = 1$, FIOs with symbols $u \in S[m; 2d]$ and (not necessarily homogeneous) phase functions of the form

$$\Phi(x,y,\theta) = \widetilde{\Phi}'(x,\theta) - y \cdot \theta,$$

fulfilling the decay condition that $\Phi - x \cdot \theta$ is in the Hörmander-class $S^1_{1,0}$, i.e.

$$\left|\partial_x^\alpha \partial_\theta^\beta \left(\Phi - x \cdot \theta\right)\right| \leq C \left\langle\theta\right\rangle^{1-|\beta|} \quad \forall x, \theta \in \mathbb{R}^d$$

and a non-degeneracy assumption related to $\det\left(D(\Phi)(x,y,\theta)\right) > \delta$ and are discussed and shown to be continuous on $L^2(\mathbb{R}^d)$ if $u \in S[0;2d]$. Later on, the treatment was generalised to symbol classes defined by arbitrary order functions, see [Asa81].

The first semiclassical result for general non-homogeneous phase-functions was shown by Asada and Fujiwara.

3.1 Theorem ([AF78]). *Assume that*

- $D(\Phi), u \in \mathcal{S}(\mathbb{R}^{2d+D})$.
- $\det\left(D(\Phi)(x,y,\theta)\right) \geq \delta > 0$ *uniformly in* $(x,y,\theta) \in \mathbb{R}^{2d+D}$.

Then $\mathcal{I}^\varepsilon(\Phi,u)$ *is continuous from* $L^2(\mathbb{R}^d)$ *into itself with* ε*-independent norm-bound*

$$\|\mathcal{I}^\varepsilon(\Phi,u)\|_{L^2 \to L^2} \leq C.$$

Since these early works, a lot of papers concerning the L^2-continuity of FIOs with real and complex valued phase functions have been published. In particular, the strong decay properties of the phase and the symbols have been alleviated, see e.g. [RS06]. A review of local and global L^2 and Sobolev continuity results is given in [Ruz].

However, the works cited there do not apply to the IVR form (0.7), because they either assume real phase functions or phase functions which are homogeneous with respect to the covariable θ. Moreover, the results do not discuss the semiclassical situation such that it is unclear how the norm of an FIO would behave upon introduction of a small parameter ε. Results closer related to specific form of IVRs only appear as auxiliary results in papers directly connected to the approximation of the unitary propagator of (1.8) and will be discussed in this context at the beginning of Part III.

4 A class of Fourier Integral Operators with complex phase

We start our discussion of Fourier-Integral Operators with a rigorous explanation for the "expansion in the overcomplete basis of coherent states", which was the starting point of the heuristic derivation of IVRs in the introduction. Before we introduce the main mathematical tool, the Fourier-Bros-Iagolnizer(FBI)-transform, we recall our notion of a coherent state

$$g^{\varepsilon,\Theta}_{(q,p)}(x) = \frac{(\det \Re\Theta)^{1/4}}{(\pi\varepsilon)^{d/4}} e^{-\Theta(x-q)^2/2\varepsilon + ip\cdot(x-q)/\varepsilon}.$$

A property among others which makes coherent states especially interesting is that they are the "best localized" wavefunctions in phase-space in the following sense: the uncertainty principle prevents that a wavefunction $\psi \in L^2(\mathbb{R}^d)$ is arbitrarily sharp localised both in position and momentum space. The best compromise is provided by Gaussian wavefunctions. More precisely, one has

4.1 Theorem ([FS97], Theorem 1.1)**.** *Let $\psi \in L^2(\mathbb{R})$ with $\|\psi\| = 1$. Then Heisenberg's inequality*

$$\langle\psi\rangle_X \, \langle\psi\rangle_P \geq \frac{\varepsilon}{2} \tag{4.1}$$

holds, where

$$\langle\psi\rangle_X = \left[\inf_{a\in\mathbb{R}} \int_{\mathbb{R}} (x-a)^2 \, |\psi(x)|^2 \, dx\right]^{\frac{1}{2}} \text{ and } \langle\psi\rangle_P = \left[\inf_{b\in\mathbb{R}} \int_{\mathbb{R}} (\xi-b)^2 \, |(\mathcal{F}^\varepsilon\psi)(\xi)|^2 \, d\xi\right]^{\frac{1}{2}}$$

denote the variance in position and momentum space. Equality in (4.1) *holds if and only if $\psi = cg^{\varepsilon,\Theta}_{(q,p)}$ for some $(q,p) \in \mathbb{R}^2$, $\Theta > 0$ and $c \in \mathbb{C}$ with $|c| = 1$.*

A multidimensional analogue of (4.1) is shown in Corollary 5.7 of [FS97]. For a multidimensional version of the equivalence between equality and a certain Gaussian shape of the wavefunction connected to the metaplectic representation, consider Proposition 4.75 in [Fol89].

4.1 The FBI-transform

The Θ-scaled semiclassical FBI-transform is defined as the overlap of the wavefunction with a coherent state. Considering Theorem 4.1 it provides a tool for the study of the microlocal structure of a wavefunction. The definition and results in this section are a collection of results and exercises in Chapter 3 of [Mar02], where the traditional semiclassical FBI-transform, which arises for $\Theta = \mathrm{id}$ is discussed. Originally, the FBI-transform was introduced in [Iag75].

4.2 Definition (FBI transform).
*For a symmetric and positive definite matrix $\Theta \in \mathbb{C}^{d\times d}$ we define the Θ-**scaled FBI transform** of $\varphi \in \mathcal{S}(\mathbb{R}^d)$ as*

$$\begin{aligned}\left[T^\varepsilon[\Theta]\,\varphi\right](q,p) &:= \frac{(\det \Re\Theta)^{1/4}}{2^{d/2}(\pi\varepsilon)^{3d/4}} \int_{\mathbb{R}^d} e^{-\overline{\Theta}(y-q)^2/2\varepsilon - ip\cdot(y-q)/\varepsilon}\varphi(y)\,dy \\ &= (2\pi\varepsilon)^{-d/2}\left\langle g^{\varepsilon,\Theta}_{(q,p)}\middle|\varphi\right\rangle_{L^2(\mathbb{R}^d)} \end{aligned} \tag{4.2}$$

*and the **inverse** Θ-**scaled FBI transform** of a function $\Phi \in \mathcal{S}(\mathbb{R}^{2d})$*

$$\begin{aligned}\left[T^\varepsilon_{\text{inv}}[\Theta]\,\Phi\right](x) &:= \frac{(\det \Re\Theta)^{1/4}}{2^{d/2}(\pi\varepsilon)^{3d/4}} \int_{\mathbb{R}^{2d}} e^{-\Theta(x-q)^2/2\varepsilon + ip\cdot(x-q)/\varepsilon}\Phi(q,p)\,dq\,dp \\ &= (2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^{2d}} g^{\varepsilon,\Theta}_{(q,p)}(x)\Phi(q,p)\,dq\,dp. \end{aligned} \tag{4.3}$$

The definition of positive definiteness for non-real matrices and some properties are recalled in the appendix. Thinking of the integral in (4.3) as a generalised sum, one immediately recognises the formal similarity to the coordinate representation in a finite basis. The second assertion of the following Proposition puts even more emphasis on this formal viewpoint:

4.3 Proposition.

1. *$T^\varepsilon[\Theta]$ and $T^\varepsilon_{\text{inv}}[\Theta]$ are continuous from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^{2d})$ and $\mathcal{S}(\mathbb{R}^{2d})$ to $\mathcal{S}(\mathbb{R}^d)$ respectively.*
2. *$T^\varepsilon[\Theta]$ extends to an isometry from $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$. Moreover, we have the reconstruction formula*
$$T^\varepsilon_{\text{inv}}[\Theta]\,T^\varepsilon[\Theta] = \text{id}_{L^2(\mathbb{R}^d)}.$$
In particular
$$T^\varepsilon[\Theta]^*|_{T^\varepsilon[\Theta]L^2(\mathbb{R}^d)} = T^\varepsilon_{\text{inv}}[\Theta]|_{T^\varepsilon[\Theta]L^2(\mathbb{R}^d)}\,.$$
3. *We have $T^\varepsilon\left[\overline{\Theta}\right]L^2(\mathbb{R}^d) = L^2(\mathbb{R}^{2d}) \cap e^{-\Theta^{-1}p^2/2\varepsilon}\mathcal{H}_{\Theta q - ip}$, where $\mathcal{H}_{\Theta q-ip}$ denotes the space of holomorphic functions with respect to $\Theta q - ip \in \mathbb{C}^d$.*

Proof.

1. $T^\varepsilon[\Theta]$ is the composition of the partial ε-scaled Fourier-transform of the Schwartz function
$$(q,y) \to (\det\Re\Theta)^{1/4}(\varepsilon\pi)^{-d/4}e^{\overline{\Theta}(y-q)^2/2\varepsilon}\varphi(y)$$
with respect to y and the multiplication with $e^{\frac{i}{\varepsilon}p\cdot q}$ and is thus continuous from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^{2d})$. Similarly, denoting the partial inverse Fourier-transform with respect to the second variable by $(\mathcal{F}^\varepsilon_2)^{-1}$, $T^\varepsilon_{\text{inv}}[\Theta]$ is given by
$$\left(T^\varepsilon_{\text{inv}}[\Theta]\,\Phi\right)(x) = (\det\Re\Theta)^{1/4}(\pi\varepsilon)^{-d/4}\int_{\mathbb{R}^d}\left[(\mathcal{F}^\varepsilon_2)^{-1}\Phi\right](q,x-q)e^{-\Theta(x-q)^2/2\varepsilon}\,dq,$$
which is the convolution with respect to the first variable of the Schwartz-class function
$$(q,x') \mapsto \left[(\mathcal{F}^\varepsilon_2)^{-1}\Phi\right](q,x'-q)$$
with a Gaussian evaluated at $x' = x$ and thus continuous from $\mathcal{S}(\mathbb{R}^{2d})$ to $\mathcal{S}(\mathbb{R}^d)$.

2. It is enough to show the property on the dense subspace $\mathcal{S}(\mathbb{R}^d)$ of $L^2(\mathbb{R}^d)$. Introducing an extra Gaussian in the inner product to make the integrals absolutely convergent and to allow for the application of Fubini's Theorem, we have

$$\begin{aligned}
&\|T^\varepsilon[\Theta]\,\varphi\|^2_{L^2(\mathbb{R}^{2d})}\\
&= \lim_{\delta\to 0}\int_{\mathbb{R}^{2d}} \exp\left(-\delta^2 p^2/2\varepsilon\right)\overline{[T^\varepsilon[\Theta]\,\varphi]\,(q,p)}\,[T^\varepsilon[\Theta]\,\varphi]\,(q,p)\;dq\,dp\\
&= \lim_{\delta\to 0}\frac{(\det\Re\Theta)^{1/2}}{2^d(\pi\varepsilon)^{3d/2}}\int_{\mathbb{R}^{4d}} \exp\left(-\delta^2 p^2/2\varepsilon\right)\overline{\varphi(y_1)}\varphi(y_2)\\
&\quad\times\exp\left(ip\cdot(y_1-y_2)/\varepsilon-\Theta(y_1-q)^2/2\varepsilon-\overline{\Theta}(y_2-q)^2/2\varepsilon\right)\;dy_1\,dy_2\,dq\,dp.
\end{aligned}$$

The p-integral is the Fourier-transform of a Gaussian and gives

$$\begin{aligned}
&\lim_{\delta\to 0}\frac{(\det\Re\Theta)^{1/2}}{2^{d/2}(\pi\varepsilon)^d}\delta^{-d}\int_{\mathbb{R}^{3d}}\overline{\varphi(y_1)}\varphi(y_2)\\
&\quad\times\exp\left(-\delta^{-2}(y_1-y_2)^2/2\varepsilon-\Theta(y_1-q)^2/2\varepsilon-\overline{\Theta}(y_2-q)^2/2\varepsilon\right)\;dy_1\,dy_2\,dq\\
&= \lim_{\delta\to 0}(2\pi\varepsilon)^{-d/2}\delta^{-d}\int_{\mathbb{R}^{2d}}\exp\left(-\delta^2(y_1-y_2)^2/2\varepsilon\right)\overline{\varphi\,(y_1)}\varphi\,(y_2)\\
&\quad\times\exp\left(-\left[\Im\Theta(\Re\Theta)^{-1}\Im\Theta+\Re\Theta\right](y_1-y_2)^2/4\varepsilon\right)\;dy_1\,dy_2,
\end{aligned}$$

where we used Lemma 11.4 from the appendix for the inner product of the Gaussians in the last expression. Using the orthogonal transformation defined by

$$\begin{pmatrix} y_1\\ y_2\end{pmatrix}=\begin{pmatrix}\hat{y}+\delta_y/2\\ \hat{y}-\delta_y/2\end{pmatrix}$$

and rescaling the integration variable δ_y with δ, we obtain

$$\begin{aligned}
&\lim_{\delta\to 0}(2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^{2d}}\exp\left(-\delta_y^2/2\varepsilon\right)\overline{\varphi\left(\hat{y}+\tfrac{\delta}{2}\delta_y\right)}\varphi\left(\hat{y}-\tfrac{\delta}{2}\delta_y\right)\\
&\quad\times\exp\left(-\delta^2\left[\Im\Theta(\Re\Theta)^{-1}\Im\Theta+\Re\Theta\right]\delta_y^2/4\varepsilon\right)\;d\hat{y}\,d\delta_y\\
&= (2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^{2d}}\exp\left(-|\delta_y|^2/2\varepsilon\right)\overline{\varphi\,(\hat{y})}\varphi\,(\hat{y})\;\;d\hat{y}\,d\delta_y=\|\varphi\|^2_{L^2(\mathbb{R}^d)}\,.
\end{aligned}$$

The reconstruction formula now follows from the polarization of the preceding identity

$$\begin{aligned}
\langle\psi|\varphi\rangle_{L^2(\mathbb{R}^d)} &= \langle T^\varepsilon[\Theta]\,\psi|T^\varepsilon[\Theta]\,\varphi\rangle_{L^2(\mathbb{R}^{2d})}\\
&= (2\pi\varepsilon)^{-d/2}\left\langle\int_{\mathbb{R}^d}\overline{g_\cdot^{\varepsilon,\Theta}(y)}\psi(y)\;dy\,\middle|\,T^\varepsilon[\Theta]\,\varphi\right\rangle_{L^2(\mathbb{R}^{2d})}\\
&= (2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^d} g^{\varepsilon,\Theta}_{(q,p)}(y)\overline{\psi(y)}[T^\varepsilon[\Theta]\,\varphi](q,p)\;dy\,dq\,dp\\
&= \int_{\mathbb{R}^d}\overline{\psi(y)}\left[(2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^{2d}} g^{\varepsilon,\Theta}_{(q,p)}(y)[T^\varepsilon[\Theta]\,\varphi](q,p)\;dq\,dp\right]dy\\
&= \langle\psi|T^\varepsilon_{\mathrm{inv}}[\Theta]\,T^\varepsilon[\Theta]\,\varphi\rangle_{L^2(\mathbb{R}^d)}\,.
\end{aligned}$$

3. In a first step, we note that $T^\varepsilon\left[\Theta\right]$ can be written as

$$(T^\varepsilon\left[\Theta\right]\varphi)(q,p) = \frac{(\det\Re\Theta)^{1/4}}{2^{d/2}(\pi\varepsilon)^{3d/4}} e^{-(\Theta)^{-1}p^2/2\varepsilon}\int_{\mathbb{R}^d} e^{-\Theta\left(q-i(\Theta)^{-1}p-y\right)^2/2\varepsilon}\varphi(y)\,dy, \tag{4.4}$$

i.e. it is the convolution of φ with a Gaussian evaluated at $z = q - i\Theta^{-1}p$ and hence continuous in $\widetilde{z} = \Theta z = \Theta q - ip$, so

$$T^\varepsilon\left[\Theta\right] L^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^{2d}) \cap e^{-\Theta^{-1}p^2/2\varepsilon}\mathcal{H}_{\Theta q - ip}.$$

Now consider $\Pi^\varepsilon(\Theta) = T^\varepsilon\left[\Theta\right]\left[T^\varepsilon\left[\Theta\right]\right]^*$, the projection onto $T^\varepsilon\left[\Theta\right] L^2(\mathbb{R}^d)$ and let $\psi \in \mathcal{S}(\mathbb{R}^{2d}) \cap e^{-\Theta^{-1}p^2/2\varepsilon}\mathcal{H}_{\Theta q-ip}$, i.e. $\psi(q,p) = e^{-\Theta^{-1}p^2/2\varepsilon}\varphi(\Theta q - ip)$ for some holomorphic function φ. We have

$$\begin{aligned}
&\left(\Pi^\varepsilon(\Theta)\psi\right)(x,\xi)\\
&= \frac{(\det\Re\Theta)^{1/2}}{2^d(\pi\varepsilon)^{3d/2}}\int_{\mathbb{R}^{3d}} e^{-\Theta(y-x)^2/2\varepsilon - i\xi\cdot(y-x)/\varepsilon - \overline{\Theta}(y-q)^2/2\varepsilon + ip\cdot(y-q)/\varepsilon}\psi(q,p)\,dq\,dp\,dy\\
&= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{-(\Re\Theta)^{-1}(\xi-p)^2/4\varepsilon - \left(\Theta(\Re\Theta)^{-1}\overline{\Theta}\right)(x-q)^2/4\varepsilon}\\
&\qquad e^{i(\xi-p)(\Re\Theta)^{-1}(\overline{\Theta}-\Theta)(x-q)/4\varepsilon + i(\xi+p)(x-q)/2\varepsilon - \Theta^{-1}p^2/2\varepsilon}\varphi(\Theta q - ip)\,dq\,dp.
\end{aligned}$$

As in the proof of assertion 2, we introduce an extra Gaussian to assure the absolute convergence of the p-integral. As the integrand is holomorphic in q, we can perform the integral transformation

$$q \mapsto q + i\Theta^{-1}(p-\xi)$$

and obtain

$$\begin{aligned}
&(2\pi\varepsilon)^d\left(\Pi^\varepsilon(\Theta)\psi\right)(x,\xi)\\
&= \lim_{\delta\to 0}\int_{\mathbb{R}^{2d}} e^{-\delta^2p^2/2\varepsilon}e^{-(\Re\Theta)^{-1}(\xi-p)^2/4\varepsilon - \left(\Theta(\Re\Theta)^{-1}\overline{\Theta}\right)(x-q-i\Theta^{-1}(p-\xi))^2/4\varepsilon}\\
&\qquad e^{i(\xi-p)(\Re\Theta)^{-1}(\overline{\Theta}-\Theta)(x-q-i\Theta^{-1}(p-\xi))/4\varepsilon + i(\xi+p)(x-q-i\Theta^{-1}(p-\xi))/2\varepsilon - \Theta^{-1}p^2/2\varepsilon}\varphi(\Theta q - i\xi)\,dq\,dp\\
&= \lim_{\delta\to 0}\int_{\mathbb{R}^{2d}} e^{-\delta^2p^2/2\varepsilon}e^{-\left(\Theta(\Re\Theta)^{-1}\overline{\Theta}\right)(x-q)^2 + i(x-q)(\Re\Theta)^{-1}\overline{\Theta}(p-\xi)/4\varepsilon}\\
&\qquad e^{i(\xi-p)(\Re\Theta)^{-1}(-\Theta)(x-q)/4\varepsilon + i(\xi+p)(x-q) + \Theta^{-1}p^2/2\varepsilon - \Theta^{-1}\xi^2/2\varepsilon - \Theta^{-1}p^2/2\varepsilon}\varphi(\Theta q - i\xi)\,dq\,dp\\
&= \lim_{\delta\to 0}\int_{\mathbb{R}^{2d}} e^{-\delta^2p^2/2\varepsilon}e^{-\left(\Theta(\Re\Theta)^{-1}\overline{\Theta}\right)(x-q)^2 + ip\cdot(x-q)/\varepsilon}e^{-\Theta^{-1}\xi^2/2\varepsilon}\varphi(\Theta q - i\xi)\,dq\,dp\\
&= (2\pi\varepsilon)^d\psi(x,\xi),
\end{aligned}$$

where the last step arises from the argument already shown previously in the proof. Hence $\psi \in \operatorname{Ran}\left(\Pi^\varepsilon(\Theta)\right) = T^\varepsilon\left[\Theta\right] L^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^{2d})$ and thus the second inclusion

$$e^{-(\Theta)^{-1}p^2/2\varepsilon}\mathcal{H}_{\Theta q - ip} \subset T^\varepsilon\left[\Theta\right] L^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^{2d}).$$

□

4.2 Two definitions of Fourier Integral Operators

Before we turn to the first definition of Fourier Integral Operators we discuss the relation between the FBI-transform and other phase-space representations. As suggested by (4.4), the FBI-transform is related to a transformation into a space of analytic functions, namely the Bargmann-transform ([Bar61]), which is defined by

$$\begin{aligned} \mathcal{B}^\varepsilon : \mathcal{S}(\mathbb{R}^d) &\to \mathcal{F}^2(\mathbb{C}^d) \\ \psi \mapsto (\mathcal{B}^\varepsilon \psi)(z) &= (\pi\varepsilon)^{-d/4} \int_{\mathbb{R}^d} e^{z^2/4\varepsilon} e^{-(z-y)^2/2\varepsilon} \psi(y)\, dy. \end{aligned} \tag{4.5}$$

$\mathcal{B}^\varepsilon$ is unitary from $L^2(\mathbb{R}^d)$ to the Fock-space $\mathcal{F}^2(\mathbb{C}^d)$ in d variables, i.e. the space of entire functions whose norm defined by the inner product

$$\langle \psi, \varphi \rangle_{\mathcal{F}^2(\mathbb{C}^d)} = (2\pi\varepsilon)^{-d} \int_{\mathbb{C}^d} \overline{\varphi(z)} \psi(z) e^{-|z|^2/2\varepsilon}\, dz$$

is finite, compare Section I.6 of [Fol89]. One of the main applications of the Bargman-transform lies in quantum-field theory. When photons are modelled, the creation and annihilation operators

$$\mathfrak{a}_j^\dagger = x - \varepsilon \partial_{x_j} \quad \text{and} \quad \mathfrak{a} = x + \varepsilon \partial_{x_j}$$

appear naturally. Using these operators, the Wick and Anti-Wick-quantisations of a polynomial symbol

$$h(z, \overline{z}) = \sum a_{\alpha\beta} z^\alpha \overline{z}^\beta$$

are given by

$$\mathrm{op}_{\mathrm{W}}^\varepsilon(h) = \sum a_{\alpha\beta} (\mathfrak{a}^\dagger)^\beta \mathfrak{a}^\alpha \quad \text{and} \quad \mathrm{op}_{\mathrm{AW}}^\varepsilon(h) = \sum a_{\alpha\beta} \mathfrak{a}^\alpha (\mathfrak{a}^\dagger)^\beta.$$

The generalisation to more general symbols $h : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C}$ with suitable growth restrictions uses the relation

$$\mathcal{B}^\varepsilon \mathfrak{a}_j^\dagger (\mathcal{B}^\varepsilon)^{-1} F(z) = z_j F(z) \quad \text{and } \mathcal{B}^\varepsilon \mathfrak{a}_j (\mathcal{B}^\varepsilon)^{-1} F(z) = 2\varepsilon \partial_{z_j} F(z) \tag{4.6}$$

for functions $F \in \mathcal{F}^2(\mathbb{C}^d)$ and the reproducing formula

$$F(z) = (2\pi\varepsilon)^{-d/2} \int e^{\overline{w} \cdot z/2} e^{-|w|^2/2\varepsilon} F(w)\, dw \qquad \forall F \in \mathcal{F}^2(\mathbb{C}^d)$$

and reads

$$\left(\mathcal{B}^\varepsilon \mathrm{op}_{\mathrm{AW}}^\varepsilon(h) (\mathcal{B}^\varepsilon)^{-1} F\right)(z) = (2\pi\varepsilon)^{-d/2} \int h(\overline{w}, w) e^{z\overline{w}/2\varepsilon} F(w) e^{-|w|^2/2\varepsilon}\, dw.$$

Retranslating this identity to $L^2(\mathbb{R}^d)$, one has

$$(\mathrm{op}_{\mathrm{AW}}^\varepsilon(h)\varphi)(x) = \frac{2^{d/2}}{(2\pi\varepsilon)^{3d/2}} \int_{\mathbb{R}^{3d}} e^{-(x-q)^2/2\varepsilon - (y-q)^2/2\varepsilon + ip\cdot(x-y)/\varepsilon} \hat{h}(q,p) \varphi(y)\, dq\, dp\, dy,$$

where $\hat{h}(q,p) = h(q+ip, q-ip)$, i.e.

$$(\mathrm{op}_{\mathrm{AW}}^\varepsilon(h)\varphi)(x) = \left(T_{\mathrm{inv}}^\varepsilon[\mathrm{id}] \circ \mathrm{M}_{\hat{h}} \circ T^\varepsilon[\mathrm{id}]\, \varphi\right)(x),$$

for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $h \in S[0; 2d]$, where $\mathrm{M}_{\hat{h}}$ stands for the multiplication operator induced by $\hat{h}$. Moreover, the Anti-Wick quantisation can be related to the Weyl-quantisation, more precisely, one has

$$\mathrm{op}^{\varepsilon}_{\mathrm{AW}}(h) = \mathrm{op}^{\varepsilon}(g),$$

where

$$g(x,\xi) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} e^{-(x-q)^2/2\varepsilon-(\xi-p)^2/2\varepsilon} \hat{h}(q,p)\, dq\, dp,$$

i.e. the Weyl-Symbol is the smoothed Anti-Wick symbol of a pseudo-differential operator. In particular, every operator which has an Anti-Wick symbol has a Weyl-symbol but the converse is in general not true.

Finally, the Anti-Wick theory provides an analogue to the duality relation (1.4) between Wigner-functions and Weyl-quantised operators by the Husimi function ([Hus40])

$$\mathcal{H}^{\varepsilon}[\varphi](q,p) = (\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \mathcal{W}^{\varepsilon}[\varphi,\varphi](x,\xi) e^{-(q-x)^2/\varepsilon-(p-\xi)^2/\varepsilon}\, dx\, d\xi = \left|T^{\varepsilon}[\mathrm{id}]\, \varphi(q,p)\right|^2, \qquad (4.7)$$

i.e.

$$\langle \mathrm{op}_{\mathrm{AW}}(h)\varphi|\varphi\rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} \hat{h}(q,p)\mathcal{H}^{\varepsilon}[\varphi](q,p)\, dq\, dp.$$

To conclude this excursus, we mention that the use of coherent states in the FBI and Bargman transform is not mandatory. A more general theory using general phase-space localized functions leads to the geometric or Berezin quantization schemes.

We will meet the creation and annihilation structure later on, when we discuss the composition of PDOs and FIOs. At this time, we have the following connection to our FIOs: in the case $\kappa = \mathrm{id}$ and $\Theta^x = \Theta^y = \mathrm{id}$ the following definition of an FIO reduces exactly to the Anti-Wick quantisation.

4.4 Definition (Anti-Wick FIO)**.** *For a canonical transformation κ, a symbol $u \in L^{\infty}(\mathbb{R}^{2d})$, and positive definite symmetric $\Theta^x, \Theta^y \in \mathbb{C}^{d\times d}$ we define the* ***semiclassical Fourier Integral Operator associated to κ with symbol*** *u as the linear operator $\mathcal{I}^{\varepsilon}_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)$, which fulfills*

$$\langle \psi | \mathcal{I}^{\varepsilon}_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)\, \varphi\rangle_{L^2(\mathbb{R}^d)} = \left\langle \left[T^{\varepsilon}[\Theta^x]\, \psi\right] \circ \kappa \middle| e^{\frac{i}{\varepsilon}S^{\kappa}} u \left[T^{\varepsilon}\left[\overline{\Theta^y}\right] \varphi\right] \right\rangle_{L^2(\mathbb{R}^{2d})} \qquad (4.8)$$

for all $\varphi, \psi \in L^2(\mathbb{R}^d)$.

The definition mirrors the idea of a basis, which is moving along the classical flow: First, the function φ is expanded in coherent states; then, the "coefficients" are weighted according to the symbol u and multiplied by a phase factor; finally, the inner product with $T^{\varepsilon}[\Theta^x]\,\psi$ corresponds to the reconstruction in basis functions, which were transformed by κ. We collect some properties of these operators in the following Lemma.

4.5 Lemma.

1. *$\mathcal{I}^{\varepsilon}_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)$ is well-defined.*

2. *$\|\mathcal{I}^{\varepsilon}_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \leq \|u\|_{L^{\infty}(\mathbb{R}^{2d})}$.*

3. *If $u \in L^1(\mathbb{R}^{2d}) \cap L^\infty(\mathbb{R}^{2d})$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have*

$$\begin{aligned}&\left(\mathcal{I}^\varepsilon_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)\, \varphi\right)(x) \\ &= \frac{(\det \Re\Theta^x)^{1/4}\,(\det \Re\Theta^y)^{1/4}}{2^{-d/2}(2\pi\varepsilon)^{3d/2}} \int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} u(q,p)\varphi(y)\; dq\, dp\, dy\end{aligned} \tag{4.9}$$

where

$$\begin{aligned}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y) := {}& S^\kappa(q,p) + \Xi^\kappa(q,p)\cdot(x - X^\kappa(q,p)) - p\cdot(y-q) \\ &+ i\Theta^x(x - X^\kappa(q,p))^2/2 + i\Theta^y(y-q)^2/2.\end{aligned} \tag{4.10}$$

Proof.

1.,2. For fixed $\varphi \in L^2(\mathbb{R}^d)$, the inner product

$$\psi \mapsto \left\langle e^{\frac{i}{\varepsilon}S^\kappa} u \left[T^\varepsilon\left[\overline{\Theta^y}\right]\varphi\right] \middle| \left[T^\varepsilon[\Theta^x]\,\psi\right]\circ\kappa \right\rangle_{L^2(\mathbb{R}^{2d})}$$

is a continuous linear form in $\psi \in L^2(\mathbb{R}^d)$ with norm bounded by $\|u\|_{L^\infty(\mathbb{R}^d)}\,\|\varphi\|_{L^2(\mathbb{R}^d)}$. Hence, by the Riesz representation theorem, there exists a unique vector $\Phi_\varphi \in L^2(\mathbb{R}^d)$ with norm bounded by $\|u\|_{L^\infty(\mathbb{R}^d)}\,\|\varphi\|_{L^2(\mathbb{R}^d)}$, which fulfills

$$\left\langle e^{\frac{i}{\varepsilon}S^\kappa} u \left[T^\varepsilon\left[\overline{\Theta^y}\right]\varphi\right] \middle| \left[T^\varepsilon[\Theta^x]\,\psi\right]\circ\kappa \right\rangle_{L^2(\mathbb{R}^{2d})} = \langle \Phi_\varphi | \psi\rangle_{L^2(\mathbb{R}^d)}$$

for all $\psi \in L^2(\mathbb{R}^d)$. Moreover the correspondence between φ and Φ_φ is linear. Thus

$$\mathcal{I}^\varepsilon_{\mathrm{AW}}(\kappa; u; \Theta^x, \Theta^y)\,\varphi := \Phi_\varphi$$

defines a linear operator with norm bounded by $\|u\|_{L^\infty(\mathbb{R}^{2d})}$.

3. The result follows by direct computation, which is presented in the proof of assertion 3. of Lemma 4.9.

□

The definition of an Anti-Wick Fourier Integral Operator via the duality relation (4.8) is very appealing, as it elucidates the microlocal structure of the operator. In this aspect, it is comparable to the relation (1.4), which explains the action of Weyl-pseudodifferential operators in a phase-space formulation. However, it also shares the same drawback of being an implicit definition. This prohibits explicit transformations, such as compositions with pseudodifferential operators and time-derivatives.

A second problem comes with the restriction to matrices Θ^x and Θ^y which are constant with respect to the variables q and p. This excludes all Initial Value Representation but the Herman-Kluk propagator. One way to circumvent this problem is to generalise the FBI-transform to non-constant matrices Θ^x and Θ^y. However, taking the first objection into account, we do not follow this approach but include the additional dependence of Θ^x and Θ^y only in the definition of Fourier Integral Operators via oscillatory integrals.

For the matrices Θ^x and Θ^y we will put two restrictions: First, we require an uniform bound from below for their real parts. If we would drop this assumption, we would include FIOs with real phase and meet the problem of caustics inherent to this class of operators. Second, we assume that they depend smoothly on q and p and that all derivatives are uniformly bounded.

4.6 Definition (Accessible width-matrices)**.** *We define the set*

$$\mathcal{C} := \left\{ \Theta \in C^\infty\left(\mathbb{R}^{2d}, \mathbb{C}^{d\times d}\right) \cap S[0;2d] \,\middle|\, \Theta^\dagger = \Theta, \exists \Theta_0 \in \mathcal{C}_{\mathrm{const}}, \Re\Theta - \Theta_0 \geq 0 \right\},$$

where

$$\mathcal{C}_{\mathrm{const}} := \left\{ \Theta \in \mathbb{R}^{d\times d} \,\middle|\, \Theta^\dagger = \Theta, \Theta > 0 \right\}.$$

In Section 10.2 we collected some properties of the matrices of $\mathcal{C}$. In particular, it is shown that every element admits a unique matrix square-root in $\mathcal{C}$ and that its inverse is in $\mathcal{C}$.

We base the definition our FIOs on the oscillatory integral expression (4.9). The phase function

$$\begin{aligned}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y) := {} & S^\kappa(q,p) + \Xi^\kappa(q,p)\cdot(x - X^\kappa(q,p)) - p\cdot(y-q) \\ & + i\Theta^x(q,p)(x - X^\kappa(q,p))^2/2 + i\Theta^y(q,p)(y-q)^2/2\end{aligned} \tag{4.11}$$

gives rise to the operator

$$L_y := \frac{1 - i\varepsilon\nabla_y\overline{\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)}}{1 + |\nabla_y\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)|^2}\cdot\nabla_y, \tag{4.12}$$

which fulfills

$$L_y e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} = e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} \tag{4.13}$$

and provides decay in the p-variable:

4.7 Lemma. *Let $u \in \mathcal{S}(\mathbb{R}^d)$. We have*

$$\left|\left(L_y^\dagger\right)^k u(x)\right| \leq M_k^y[\Theta^x,\Theta^y,\varepsilon]\,\langle p - i\Theta^y(q,p)(y-q)\rangle^{-k}\sum_{|\alpha|\leq k}\left|\partial_y^\alpha u(x)\right|.$$

The proof of the Lemma is found in the appendix. We define:

4.8 Definition (FIO with complex phase)**.**
For a canonical transformation κ, a symbol $u \in S[(+\infty, m_p);(3d,d)]$, $\Theta^x, \Theta^y \in \mathcal{C}$, $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and an integer $k > m_p + d$, we define the ***semiclassical Fourier Integral Operator associated to κ with symbol*** *u as*

$$\left(\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi\right)(x) := (2\pi\varepsilon)^{-3d/2}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)}(L_y^\dagger)^k[u(x,y,q,p)\varphi(y)]\,dq\,dp\,dy$$

where the phase function Φ^κ is given by (4.11) *and the operator L_y is defined in* (4.12)*.*

As presented, the oscillatory integral does not generalise Definition 4.4 as we made stronger regularity assumptions with respect to (q,p). Whereas the duality relation (4.8) only requires $u \in L^\infty(\mathbb{R}^{2d})$, the symbols in $S[+\infty;4d]$ are smooth with respect to (q,p). However, we will never use this regularity in Part II, such that all results including the continuity results Proposition 4.10 and Theorem 4.11 hold if the regularity assumption with respect to (q,p) is reduced to measurability. For sake of a simpler representation we decided not to provide the full generality here.

Besides the variation of the matrices Θ^x and Θ^y, there is another main difference to the Anti-Wick Fourier Integral operators: The symbols are allowed to depend on x and y. Considering that we want to apply pseudodifferential operators to the FIOs, the necessity for the x-dependence is immediately clear. The second reason for the x and y dependence lies in the dependence of Θ^x and Θ^y on q and p, which will be considered as part of the symbol later on, compare Section 4.4.1.

We have the following basic properties of our FIOs:

4.9 Lemma.

1. *$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ is well-defined.*
2. *If $\sigma \in \mathcal{S}(\mathbb{R}^{2d})$ with $\sigma(0,0) = 1$, we have*
$$[\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\,\varphi]\,(x) = \lim_{\lambda\to+\infty} \left[\mathcal{I}^\varepsilon\left(\kappa; u^\lambda_\sigma; \Theta^x, \Theta^y\right)\varphi\right](x),$$
where $u^\lambda_\sigma := \sigma(q/\lambda, p/\lambda)u(x,y,q,p) \in S[(+\infty, -\infty); (2d, 2d)]$. The convergence is locally uniform with respect to x.
3. *If $u \in S[+\infty; 2d]$ and $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$, we have*
$$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) = 2^{-d/2}\left(\det \Re\Theta^x \det \Re\Theta^y\right)^{-\frac{1}{4}} \mathcal{I}^\varepsilon_{\text{AW}}(\kappa; u; \Theta^x, \Theta^y)\,.$$

Proof.

1. We have to show the convergence of the integral and the independence of the choice of k. Let m such that $u \in S[(+\infty, m, m, m_p); (d, d, d, d)]$. By Lemma 4.7 we have
$$\begin{aligned}&(2\pi\varepsilon)^{3d/2} \left|\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\,\varphi(x)\right| \\ &\le M^y_k[\Theta^x, \Theta^y; \varepsilon] \sum_{\substack{|\alpha|\le k\\ \beta\le\alpha}} \binom{\alpha}{\beta} \int_{\mathbb{R}^{3d}} \left| e^{\frac{i}{\varepsilon}\Phi^\kappa} \frac{\partial^\beta_y u(x,y,q,p)}{\langle p - i\Theta^y(y-q)\rangle^k} \partial^{\alpha-\beta}_y \varphi(y)\right| \,dq\,dp\,dy\end{aligned}$$
Now every integrand is bounded by
$$e^{-\Theta^y_0(y-q)^2/2\varepsilon} \left| \frac{\partial^\beta_y u(x,y,q,p)}{(\langle y\rangle\langle q\rangle)^m \langle p\rangle^{m_p}} \frac{(\langle y\rangle\langle q\rangle)^m\langle p\rangle^k}{\langle p - i\Theta^y(y-q)\rangle^k \langle p\rangle^{k-m_p}} \partial^{\alpha-\beta}_y\varphi(y)\right|$$
$$\begin{aligned}&\le e^{-\Theta^y_0(y-q)^2/2\varepsilon} \\ &\quad\times 2^{k+m} \left\| \frac{\partial^\beta_y u(x,y,q,p)}{(\langle y\rangle\langle q\rangle)^m\langle p\rangle^{m_p}}\right\|_{L^\infty_{(y,q,p)}} \left| \frac{\langle y\rangle^{2m}\langle q-y\rangle^m \langle\Theta^y(y-q)\rangle^k}{\langle p\rangle^{k-m_p}} \partial^{\alpha-\beta}_y\varphi(y)\right|\end{aligned}$$
where we used $\langle x+y\rangle \le 2\langle x\rangle\langle y\rangle$. Now
$$\left\| \frac{\partial^\beta_y u(x,y,q,p)}{(\langle y\rangle\langle q\rangle)^m\langle p\rangle^{m_p}}\right\|_{L^\infty_{(y,q,p)}} < \infty, \qquad \left\|\langle p\rangle^{m_p-k}\right\|_{L^1_p} < \infty,$$
$$\left\|\langle q-y\rangle^m \left\langle \|\Theta^y\|_{L^\infty(\mathbb{R}^{2d})}(q-y)\right\rangle^k e^{-\Theta^y_0(y-q)^2/2\varepsilon}\right\|_{L^1_q} < \infty \qquad \text{and}$$
$$\left\|\langle y\rangle^{2m}\,\partial^{\alpha-\beta}_y\varphi(y)\right\|_{L^1_y} < \infty,$$

so we have the convergence of the integral. The independence of k is clear because of (4.13).

2. We have

$$\begin{aligned}
&\lim_{\lambda\to\infty}\left[\mathcal{I}^\varepsilon\left(\kappa; u_\sigma^\lambda; \Theta^x, \Theta^y\right)\varphi\right](x)\\
&= \lim_{\lambda\to\infty}\frac{1}{(2\pi\varepsilon)^{3d/2}}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa} u(x,y,q,p)\sigma(q/\lambda,p/\lambda)\varphi(y)\, dq\, dp\, dy\\
&= \lim_{\lambda\to\infty}\frac{1}{(2\pi\varepsilon)^{3d/2}}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa} \sigma(q/\lambda,p/\lambda)\left(L_y^\dagger\right)^k [u(x,y,q,p)\varphi(y)]\; dq\, dp\, dy\\
&= \frac{1}{(2\pi\varepsilon)^{3d/2}}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa} \lim_{\lambda\to\infty}\sigma(q/\lambda,p/\lambda)\left(L_y^\dagger\right)^k [u(x,y,q,p)\varphi(y)]\; dq\, dp\, dy\\
&= \left[\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\,\varphi\right](x),
\end{aligned}$$

where we used dominated convergence for the exchange of the limit and the integral. The local uniformity of the limit follows from the estimates in the proof of assertion 1.

3. We have to show that $2^{d/2}\left(\det\Re\Theta^x\det\Re\Theta^y\right)^{\frac14}\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ fulfills (4.8). By the density of $\mathcal{S}(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$, it is enough to prove the identity on $\mathcal{S}(\mathbb{R}^d)$. We choose a function σ as before. By the estimates in the proof of assertion 1., the use of dominated convergence to exchange the limit and the integral is justified:

$$\begin{aligned}
&(2\pi\varepsilon)^{3d/2}\left\langle\psi|\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\,\varphi\right\rangle_{L^2(\mathbb{R}^d)}\\
&= \lim_{\lambda\to\infty}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} u_\sigma^\lambda(q,p)\varphi(y)\; dq\, dp\, dy\right]\overline{\psi(x)}\; dx\\
&= \lim_{\lambda\to\infty}\int_{\mathbb{R}^{2d}}\overline{\int_{\mathbb{R}^d} e^{-i\Xi^\kappa(q,p)\cdot(x-X^\kappa(q,p))/\varepsilon} e^{-\overline{\Theta^x}(x-X^\kappa(q,p))^2/2\varepsilon}\psi(x)\, dx} \qquad (4.14)\\
&\qquad \left[e^{iS^\kappa(q,p)/\varepsilon} u_\sigma^\lambda(q,p)\int_{\mathbb{R}^d} e^{-ip\cdot(y-q)/\varepsilon} e^{-\Theta^y(y-q)^2/2\varepsilon}\varphi(y)\; dy\right]\; dq\, dp\\
&= \left(\frac{(\det\Re\Theta^x\Re\Theta^y)^{1/4}}{2^{-d/2}(2\pi\varepsilon)^{3d/2}}\right)^{-1}\lim_{\lambda\to\infty}\left\langle [T^\varepsilon[\Theta^x]\,\psi]\circ\kappa\middle| e^{iS^\kappa/\varepsilon}u_\sigma^\lambda\left[T^\varepsilon\left[\overline{\Theta^y}\right]\varphi\right]\right\rangle_{L^2(\mathbb{R}^{2d})}.
\end{aligned}$$

Now the integrand of the (q,p) integral in (4.14) is dominated by

$$\|T^\varepsilon[\Theta^x]\,\psi\|_{L^\infty(\mathbb{R}^{2d})}\;\|u\|_{L^\infty(\mathbb{R}^{2d})}\;\left|\left(T^\varepsilon\left[\overline{\Theta^y}\right]\varphi\right)(q,p)\right|,$$

which is in $\mathcal{S}(\mathbb{R}^{2d})$ with respect to (q,p) and another application of dominated convergence concludes the proof.

□

4.3 Central results on Fourier Integral Operators

We have two central continuity results for our operators. The first one considers their action on Schwartz-spaces:

4.10 Proposition. *For $u \in S[+\infty; 4d]$, $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ is continuous from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^d)$.*

In particular, this means that the composition of pseudodifferential operators and a Fourier Integral Operators is well-defined as the composition of operators on $\mathcal{S}(\mathbb{R}^d)$.

The main purpose of the Fourier Integral Operators is to approximate the unitary group of the time-dependent Schrödinger equation. A minimal condition for such a property to hold is the boundedness as operators from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. We have:

4.11 Theorem. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[0;4d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$ with lower bounds Θ_0^x and Θ_0^y. Then $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ can be uniquely extended to a bounded operator from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$ and we have the ε-independent bound*

$$
\begin{aligned}
\|\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\|_{L^2\to L^2} &\le C \left\langle \|\Theta^x - \Theta_0^x\|_{L^\infty(\mathbb{R}^{2d})} \right\rangle^{4d+1} \left\langle \|\Theta^y - \Theta_0^y\|_{L^\infty(\mathbb{R}^{2d})} \right\rangle^{4d+1} \qquad (4.15)\\
&\times \left(1 + \frac{1}{\left(\min(1, \lambda^x, \lambda^y)^{(4d+1)/4} \eta^2_{[\kappa,\Theta^x,\Theta^y]}\right)} \right) \frac{\|u\|_{W^{4d+1,\infty}_{(x,y)} L^\infty_{(q,p)}}}{\det\left(\Re\Theta^x \Re\Theta^y\right)^{\frac{1}{4}}},
\end{aligned}
$$

where

$$
\lambda^{x/y} = \left\| \left(\Theta_0^{x/y}\right)^{-1} \right\|^{-1}, \quad \eta_{[\kappa,\Theta^x,\Theta^y]} = \min\left(c_{\Lambda[\Theta_0^y]}, c_{\Lambda[\Theta_0^x]\circ\kappa} \right)
$$

and the the canonical transformation $\Lambda[\Theta]$ is given by

$$
\Lambda[\Theta](q,p) = \begin{pmatrix} (\Theta)^{\frac{1}{2}} & \\ & (\Theta)^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}.
$$

We recall that c_κ is the lower Lipschitz-constant for a canonical transformation κ, compare Proposition 2.3. With respect to IVRs on the Ehrenfest-timescale, we mention the following fact, which follows directly from the norm bound: if all derivatives of Θ^x admit an upper bound, which shows the asymptotic behaviour $\varepsilon^{-\rho}$ for $\varepsilon \to 0$ and the lower bound on Θ^x decreases like ε^ρ, the norm bound is dominated by $C(\rho')\varepsilon^{-\rho'}$, where $\rho' > 0$ can be made arbitrary small if ρ is chosen small enough.

A related result shows that symbols, which carry certain factors are small with respect to ε.

4.12 Corollary. *Let κ a canonical transformation of class $\mathcal{B}$, $u \in S[0;4d]$, $\Theta^x, \Theta^y \in \mathcal{C}$ and $\alpha, \beta \in \mathbb{N}^d$. We have*

$$
\begin{aligned}
&\left\| \mathcal{I}^\varepsilon\left(\kappa; (x - X^\kappa(q,p))^\alpha (y-q)^\beta u; \Theta^x, \Theta^y\right) \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \qquad (4.16)\\
&\le C[M_0^\kappa, \Theta^x, \Theta^y] \varepsilon^{\frac{|\alpha|+|\beta|}{2}} \|u\|_{W^{4d+1,\infty}_{(x,y)} L^\infty_{(q,p)}}.
\end{aligned}
$$

Before we turn to the proofs of these results, we address two more issues: The duality definition (4.8) of an FIO suggests that the FIO acts along the canonical transformation κ. The first part of the following Proposition shows that the action of the FIO on coherent states is actually concentrated along the graph of κ, whereas the second assertion shows that we can express the identity operator by a large class of FIOs.

4.13 Proposition.

1. *Let $u \in S[+\infty; 2d]$, i.e. independent of x and y and smooth. We have*

$$\lim_{\varepsilon\to 0} \left\langle g^{\varepsilon,\overline{\Theta^x}(q_0,p_0)}_{\kappa(q_0,p_0)} \middle| \mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\, g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)} \right\rangle_{L^2(\mathbb{R}^d)} = C[\kappa; \Theta^x; \Theta^y] u(q_0, p_0), \tag{4.17}$$

where $C[\kappa; \Theta^x; \Theta^y] \neq 0$ and

$$\lim_{\varepsilon\to 0} \left\langle g^{\varepsilon,\overline{\Theta^x}(q_0,p_0)}_{(q',p')} \middle| \mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\, g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)} \right\rangle_{L^2(\mathbb{R}^d)} = 0,$$

if $(q', p') \neq \kappa(q_0, p_0)$.

2. *Let $\Theta^x, \Theta^y \in \mathcal{C}$ be p-independent. We have*

$$\mathcal{I}^\varepsilon(\mathrm{id}; u[\Theta^x, \Theta^y]; \Theta^x, \Theta^y) = \mathrm{id},$$

where

$$u[\Theta^x, \Theta^y](x) = (2\pi\varepsilon)^{d/2} \left[\int_{\mathbb{R}^d} e^{-(\Theta^x(q)+\Theta^y(q))(q-x)^2/2\varepsilon}\, dq \right]^{-1}.$$

In particular, if Θ^x and Θ^y are constant with respect to q and p, we have

$$\mathcal{I}^\varepsilon\Big(\mathrm{id}; \det(\Theta^x + \Theta^y)^{\frac{1}{2}}; \Theta^x, \Theta^y\Big) = \mathrm{id}.$$

The second part of the results shows that the norm bound of Lemma 4.5 and the one of Theorem 4.11 are not optimal. For arbitrary positive definite symmetric $\Theta^x, \Theta^y \in \mathbb{C}^{d\times d}$ it provides

$$1 = \|\mathrm{id}\| = \|\mathcal{I}^\varepsilon(\mathrm{id}; u[\Theta^x, \Theta^y]; \Theta^x, \Theta^y)\| \leq 2^{-d/2} \frac{\det(\Theta^x + \Theta^y)^{\frac{1}{2}}}{\det(\Re\Theta^x)^{\frac{1}{4}} \det(\Re\Theta^y)^{\frac{1}{4}}},$$

but the upper bound goes to infinity if $\Theta^x = \lambda\,\mathrm{id}$ and $\lambda \to \infty$.

Proof.

1. By Lemma 11.4 in the appendix, the inner product equals

$$\begin{aligned} &\frac{1}{2^{d/2}(2\pi\varepsilon)^d} \int u(q,p) e^{\frac{i}{\varepsilon}S^\kappa(q,p)} \left(\det(\Re\Theta^x(q,p))(\det(\Re\Theta^y(q,p))\right)^{-\frac{1}{4}} \\ &\qquad \left\langle g^{\varepsilon,\overline{\Theta^x}(q_0,p_0)}_{(q',p')} \middle| g^{\varepsilon,\Theta^x(q,p)}_{\kappa(q,p)} \right\rangle_{L^2(\mathbb{R}^d)} \left\langle g^{\varepsilon,\overline{\Theta^y}(q,p)}_{(q,p)} \middle| g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)} \right\rangle_{L^2(\mathbb{R}^d)} dq\, dp \\ &= \frac{2^{-d/2}}{(\pi\varepsilon)^d} \int \frac{\det(\Re\Theta^x(q_0,p_0))^{\frac{1}{4}} \det(\Re\Theta^y(q_0,p_0))^{\frac{1}{4}}\, e^{\frac{i}{\varepsilon}\Omega^\kappa(q',p',q_0,p_0,q,p)}}{\det(\Theta^x(q,p) + \Theta^x(q_0,p_0))^{\frac{1}{2}} \det(\Theta^y(q,p) + \Theta^y(q_0,p_0))^{\frac{1}{2}}} u(q,p)\, dq\, dp, \end{aligned}$$

where

$$\begin{aligned}
&\Omega^\kappa(q',p',q_0,p_0,q,p) = S^\kappa(q,p)\\
&+ (q-q_0)(p+p_0)/2\\
&+ i\Theta^y(q,p)\,(q_0-q)\cdot\left(\Theta^y(q_0,p_0)+\Theta^y(q,p)\right)^{-1}\Theta^y(q_0,p_0)\,(q_0-q)\,/2\\
&+ i\,(p_0-p)\cdot\left(\Theta^y(q_0,p_0)+\Theta^y(q,p)\right)^{-1}(p_0-p)\,/2\\
&+ i(p-p_0)\cdot\left(\Theta^y(q_0,p_0)+\Theta^y(q,p)\right)^{-1}(\Theta^y(q_0,p_0)-\Theta^y(q,p))(q-q_0)/2\\
&\\
&-(q'-X^\kappa(q,p))(p'+\Xi^\kappa(q,p))\\
&+ i\Theta^x(q_0,p_0)\left(X^\kappa(q,p)-q'\right)\cdot\left(\Theta^x(q_0,p_0)+\Theta^x(q,p)\right)^{-1}\Theta^x(q,p)\left(X^\kappa(q,p)-q'\right)/2\\
&+ i\left(\Xi^\kappa(q,p)-p'\right)\cdot\left(\Theta^x(q_0,p_0)+\Theta^x(q,p)\right)^{-1}\left(\Xi^\kappa(q,p)-p'\right)/2\\
&+ i(p'-\Xi^\kappa(q,p))\cdot\left(\Theta^x(q_0,p_0)+\Theta^x(q,p)\right)^{-1}(\Theta^x(q_0,p_0)-\Theta^x(q,p))(q'-X^\kappa(q,p))/2.
\end{aligned}$$

We want to calculate the stationary points of the phase function Ω^κ. Obviously, the conditions

$$(q,p)=(q_0,p_0) \text{ and } \kappa(q,p)=(q',p')$$

yield

$$\Im\Omega(q',p',q_0,p_0,q,p)=0 \text{ and } (\nabla_{(q,p)}\Re\Omega)(q',p',q_0,p_0,q,p)=0.$$

Moreover, they are the only stationary points. Assume that

$$\Im\Omega(q',p',q_0,p_0,q_*,p_*)=0$$

with $(q_*,p_*,\kappa(q_*,p_*))\neq(q_0,p_0,q',p')$. In this case we have

$$\Im\Omega(q',p',q_0,p_0,q_*,p_*)=0\quad\forall\varepsilon>0,$$

i.e.

$$\left|e^{\frac{i}{\varepsilon}\Omega(q',p',q_0,p_0,q_*,p_*)}\right|=1\quad\forall\varepsilon>0,$$

in contradiction to

$$\begin{aligned}
&\left|\left\langle g^{\varepsilon,\overline{\Theta^y(q_*,p_*)}}_{(q_*,p_*)}\middle|g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle_{L^2(\mathbb{R}^d)}\right|\left|\left\langle g^{\varepsilon,\Theta^x(q_*,p_*)}_{(q',p')}\middle|g^{\varepsilon,\overline{\Theta^y(q_*,p_*)}}_{\kappa(q_*,p_*)}\right\rangle_{L^2(\mathbb{R}^d)}\right|\\
&\le Ce^{-\Theta_0^y(q_*-q_0)^2/8\varepsilon}e^{-(\Theta_0^y)'(p_*-p_0)^2/8\varepsilon}e^{-\Theta_0^x(q'-X^\kappa(q_*,p_*))^2/8\varepsilon}e^{-(\Theta_0^x)'(p'-\Xi^\kappa(q_*,p_*))^2/8\varepsilon}\underset{\varepsilon\to0}{\longrightarrow}0,
\end{aligned}$$

where $(\Theta_0^y)'$ and $(\Theta_0^x)'$ are lower bounds for $\Re\left(\Theta^y\right)^{-1}$ and $\Re\left(\Theta^x\right)^{-1}$ respectively.

We choose $\sigma\in C_0^\infty(\mathbb{R}^{2d})$ with $\sigma=1$ in an neighborhood of (q_0,p_0) and split the integral into

$$\left\langle g^{\varepsilon,\overline{\Theta^x(q_0,p_0)}}_{(q',p')}\middle|\mathcal{I}^\varepsilon(\kappa;\sigma u;\Theta^x,\Theta^y)\,g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle_{L^2(\mathbb{R}^d)}\tag{4.18}$$

$$+\left\langle g^{\varepsilon,\overline{\Theta^x(q_0,p_0)}}_{(q',p')}\middle|\mathcal{I}^\varepsilon(\kappa;(1-\sigma)u;\Theta^x,\Theta^y)\,g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle_{L^2(\mathbb{R}^d)}.\tag{4.19}$$

Now (4.19) is bounded from above by

$$C(2\pi\varepsilon)^{-d}\,\|1-\sigma\|_{L^\infty(\mathbb{R}^{2d})}\int_{\operatorname{supp}(1-\sigma)}|u(q,p)|\,e^{-\Theta_0^y(q-q_0)^2/8\varepsilon}e^{-(\Theta_0^y)'(p-p_0)^2/8\varepsilon}\,dq\,dp$$

and thus exponentially small in ε, so we only have to consider the integral over the support of σ. Similarly, if $(q', p') \neq \kappa(q_0, p_0)$, the imaginary part of the phase does not vanish on the compact set $\operatorname{supp}(\sigma)$ and we have a bound of the form

$$|(4.18)| \leq \|u\|_{L^1(\operatorname{supp}\sigma)}\, e^{-C_0/\varepsilon}(\pi\varepsilon)^{-d}.$$

In the case $(q', p') = \kappa(q_0, p_0)$ we have a stationary point of the phase function which yields a zeroth-order contribution of the integral by the stationary phase Theorem 7.7.5 in [Hör83]. We have, dropping the arguments (q_0, p_0),

$$\operatorname{Hess}_{(q,p)}\Omega^\kappa = \frac{i}{2}\begin{pmatrix}\Theta^y & 0\\ 0 & (\Theta^y)^{-1}\end{pmatrix} + \frac{i}{2}\,(F^\kappa)^\dagger \begin{pmatrix}\Theta^x & 0\\ 0 & (\Theta^x)^{-1}\end{pmatrix} F^\kappa$$

at the stationary point, so

$$\lim_{\varepsilon\to 0}\left\langle g^{\varepsilon,\overline{\Theta^x(q_0,p_0)}}_{\kappa(q_0,p_0)}, \mathcal{I}^\varepsilon(\kappa;\sigma u;\Theta^x,\Theta^y)\, g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle = C[\kappa;\Theta^x(q_0,p_0);\Theta^y(q_0,p_0)]u(q_0,p_0),$$

with the non-vanishing constant

$$C[\kappa;\Theta^x;\Theta^y] = 2^{2d}\frac{\det\left(\Re\Theta^x\right)^{\frac14}\left(\Re\Theta^y\right)^{\frac14}}{\det\left(\Theta^x\right)^{\frac12}\det\left(\Theta^y\right)^{\frac12}}$$
$$\det\left(\begin{pmatrix}\Theta^y & 0\\ 0 & (\Theta^y)^{-1}\end{pmatrix} + (F^\kappa)^\dagger\begin{pmatrix}\Theta^x & 0\\ 0 & (\Theta^x)^{-1}\end{pmatrix}F^\kappa\right)^{-\frac12}.$$

2. For $\varphi \in \mathcal{S}(\mathbb{R}^d)$ we have

$$\begin{aligned}&\left(\mathcal{I}^\varepsilon(\mathrm{id};1;\Theta^x,\Theta^y)\,\varphi\right)(x)\\ &= (2\pi\varepsilon)^{-3d/2}\int_{\mathbb{R}^{3d}} e^{-\frac{i}{\varepsilon}p\cdot(x-y)}e^{-(\Theta^y(q)+\Theta^x(q))(y-q)^2/2\varepsilon}\varphi(y)\;dy\,dp\,dq\end{aligned}$$

Now the y and the q integral constitute a Fourier-inversion applied to the Schwartz-class function $\varphi e^{-(\Theta^x(q)+\Theta^y(q))(q-\cdot)^2/2\varepsilon}$ and we get

$$\left(\mathcal{I}^\varepsilon(\mathrm{id};1;\Theta^x,\Theta^y)\,\varphi\right)(x) = (2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^d} e^{-(\Theta^y(q)+\Theta^x(q))(x-q)^2/2\varepsilon}\;dq\;\varphi(x).$$

□

4.4 Proofs

We give the proofs of the continuity results.

4.4.1 Reduction to a generic case

The discussion of the continuity on Schwartz-spaces and the boundedness on $L^2(\mathbb{R}^d)$ can be restricted to the simpler case of $\varepsilon = 1$ and $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$.

4.14 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[m; 4d]$ and $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$, i.e. real symmetric and positive definite. Defining*

$$\begin{aligned} \kappa^{(\varepsilon)}(q,p) &:= \kappa(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)/\sqrt{\varepsilon}, \\ S^{\kappa^{(\varepsilon)}}(q,p) &:= S^{\kappa}(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)/\varepsilon, \\ u^{(\varepsilon)}(x,y,q,p) &:= u(\sqrt{\varepsilon}x, \sqrt{\varepsilon}y, \sqrt{\varepsilon}q, \sqrt{\varepsilon}p) \quad \text{and} \\ (D[\varepsilon]\varphi)(y) &:= \varepsilon^{d/4}\varphi(\sqrt{\varepsilon}y). \end{aligned}$$

we have

1. *$\kappa^{(\varepsilon)}$ is a canonical transformation of class $\mathcal{B}$ with inverse $(\kappa^{-1})^{(\varepsilon)}$.*
2. *$F^{\kappa^{(\varepsilon)}}(q,p) = F^{\kappa}(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)$ and thus $c_\kappa = c_{\kappa^{(\varepsilon)}}$, $C_\kappa = C_{\kappa^{(\varepsilon)}}$ and $M_0^{\kappa^{(\varepsilon)}} = M_0^{\kappa}$.*
3. *$S^{\kappa^{(\varepsilon)}}$ is an action associated to $\kappa^{(\varepsilon)}$.*
4. *$u^{(\varepsilon)} \in S^{-1/2}[m; 4d]$ and*
$$\left\| u^{(\varepsilon)} \right\|_{W^{4d+1,\infty}_{(x,y)} L^{\infty}_{(q,p)}} = \sum_{|\alpha| \le 4d+1} \varepsilon^{|\alpha|/2} \left\| \partial^{\alpha}_{(x,y)} u \right\|_{L^{\infty}(\mathbb{R}^{4d})} \tag{4.20}$$
if $u \in S[0; 4d]$.
5. *$D[\varepsilon]$ is continuous from $\mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d)$ and unitary from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$ with adjoint $(D[\varepsilon])^* = D[\varepsilon^{-1}]$.*
6. *$\mathcal{I}^{\varepsilon}(\kappa; u; \Theta^x, \Theta^y) = (D[\varepsilon])^* \circ \mathcal{I}^1\big(\kappa^{(\varepsilon)}; u^{(\varepsilon)}; \Theta^x, \Theta^y\big) \circ D[\varepsilon]$.*

Proof.

1.,2. We have
$$\left((\kappa^{-1})^{(\varepsilon)} \circ \kappa^{(\varepsilon)}\right)(q,p) = \left(\kappa^{-1} \circ \kappa\right)(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)/\sqrt{\varepsilon} = (q,p)$$
and
$$\partial^{\alpha}_{(q,p)} \kappa^{(\varepsilon)}(q,p) = \varepsilon^{\frac{|\alpha|-1}{2}} \left(\partial^{\alpha}_{(q,p)}\kappa\right)(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p).$$
Hence the statements 1. and 2. follow.

3. We have
$$\begin{aligned} S_q^{\kappa^{(\varepsilon)}}(q,p) &= S_q^{\kappa}(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)/\sqrt{\varepsilon} \\ &= -(\sqrt{\varepsilon}p)/\sqrt{\varepsilon} + X_q^{\kappa}(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)\Xi^{\kappa}(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)/\sqrt{\varepsilon} \\ &= -p + X_q^{\kappa^{(\varepsilon)}}(q,p)\Xi^{\kappa^{(\varepsilon)}}(q,p) \end{aligned}$$
and an analogous computation for $S_p^{\kappa^{(\varepsilon)}}(q,p)$.

4. The assertions follow immediately from the chain rule.

5. The $\mathcal{S}$-properties of the dilation operator $D[\varepsilon]$ is due to the chain rule, whereas the unitarity follows from the transformation theorem.

6. We have

$$\Phi^\kappa(\sqrt{\varepsilon}x, \sqrt{\varepsilon}y, \sqrt{\varepsilon}q, \sqrt{\varepsilon}p; \Theta^x, \Theta^y)/\varepsilon = \Phi^{\kappa^{(\varepsilon)}}(x, y, q, p; \Theta^x, \Theta^y)$$

and thus

$$\begin{aligned}
&(\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y))(x) \\
&= (2\pi\varepsilon)^{3d/2} \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} \sigma(q/\lambda, p/\lambda) u(x, y, q, p)\varphi(y)\, dq\, dp\, dy \\
&= (2\pi)^{3d/2} \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa(x,\sqrt{\varepsilon}y,\sqrt{\varepsilon}q,\sqrt{\varepsilon}p;\Theta^x,\Theta^y)} \sigma^{(\varepsilon)}(q/\lambda, p/\lambda) u(x, \sqrt{\varepsilon}y, \sqrt{\varepsilon}q, \sqrt{\varepsilon}p)\varphi(\sqrt{\varepsilon}y)\, dq\, dp\, dy \\
&= \left((D[\varepsilon])^* \circ \mathcal{I}^1\left(\kappa^{(\varepsilon)}; u^{(\varepsilon)}; \Theta^x, \Theta^y\right) \circ D[\varepsilon]\varphi\right)(x)
\end{aligned}$$

where $\sigma^{(\varepsilon)}(q, p) := \sigma(\sqrt{\varepsilon}q, \sqrt{\varepsilon}p)$ fulfills the assumptions of Lemma 4.9.

□

Combining statements 4.–6., we see that $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ fulfills the continuity statements of Proposition 4.10 and Theorem 4.11 if and only if $\mathcal{I}^1\left(\kappa^{(\varepsilon)}; u^{(\varepsilon)}; \Theta^x, \Theta^y\right)$ fulfills them. Moreover, we see that due to (4.20), the rescaling induces a slightly stronger bound than the one stated such that we have an ε-independent norm-bound even for $u \in S^{1/2}[0; 4d]$. This observation is fundamental for the reduction to arbitrary Θ^x and Θ^y.

4.15 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[m; 4d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$ with lower bounds Θ^x_0 and Θ^y_0. Defining*

$$v^\varepsilon = w\left(\varepsilon^{-\frac{1}{2}}(x - X^\kappa(q, p)), \varepsilon^{-\frac{1}{2}}(y - q), q, p\right) u,$$

with

$$w(x, y, q, p) = \exp\left[-\left[(\Theta^x(q, p) - \Theta^x_0)^{\frac{1}{2}}\, x\right]^2/2\right] \exp\left[-\left[(\Theta^y(q, p) - \Theta^y_0)^{\frac{1}{2}}\, y\right]^2/2\right]$$

we have

1. *$v^\varepsilon \in S^{1/2}[m; 4d]$ and*

$$\sum_{|\alpha|\le 4d+1} \varepsilon^{\frac{|\alpha|}{2}} \left\|\partial^\alpha_{(x,y)} v^\varepsilon\right\|_{L^\infty(\mathbb{R}^{4d})} \le C[\Theta^x, \Theta^y]\, \|u\|_{W^{4d+1,\infty}_{(x,y)} L^\infty_{(q,p)}}$$

for $u \in S[0; 4d]$, where

$$C[\Theta^x, \Theta^y]) = C\left\langle\left\|\Theta^x - \Theta^x_0\right\|\right\rangle^{|\alpha|} \left\langle\left\|\Theta^y - \Theta^y_0\right\|\right\rangle^{|\alpha|}.$$

2. *$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) = \mathcal{I}^\varepsilon(\kappa; v^\varepsilon; \Theta^x_0, \Theta^y_0)$.*

In particular it is sufficient to prove Proposition 4.10 and Theorem 4.11 for $\Theta_0^y, \Theta_0^x \in \mathcal{C}_{\text{const}}$.

Proof. We have

$$\begin{aligned}
&\partial^\alpha_{(x,y)} w(x,y,q,p) \\
&= w(x,y,q,p) \sum_{k=1}^{|\alpha|} \left(-\frac{1}{2}\right)^k \sum_{\substack{\alpha_1+\ldots+\alpha_k=\alpha \\ |\alpha_j|\geq 1}} \prod_{j=1}^{k} \partial^{\alpha_j}_{(x,y)} \left\{ \left(\Theta^x(q,p) - \Theta^x_0\right) x^2 + \left(\Theta^y(q,p) - \Theta^y_0\right) y^2 \right\}
\end{aligned}$$

by Fáa di Bruno's formula (11.1). For the terms in the product, we have

$$\partial^\beta_x \left\{ \left(\Theta^x(q,p) - \Theta^x_0\right) x^2 \right\} = \begin{cases} 2\left[\left(\Theta^x(q,p) - \Theta^x_0\right) x\right]_j & \text{if } \beta = e_j \\ 2\left[\left(\Theta^x(q,p) - \Theta^x_0\right)\right]_{jk} & \text{if } \beta = e_j + e_k \\ 0 & \text{if } |\beta| \geq 3 \end{cases}$$

and thus

$$\begin{aligned}
&\left| w(x,y,q,p) \partial^\beta_x \left\{ \left(\Theta^x(q,p) - \Theta^x_0\right) x^2 \right\} \right| \\
&\leq \begin{cases} \left\| x e^{-x^2/2} \right\|_{L^\infty(\mathbb{R}^{2d})} \left\| \left(\Theta^x(q,p) - \Theta^x_0\right)^{\frac{1}{2}} \right\| & \text{if } |\beta| = 1 \\ \left\| e^{-x^2/2} \right\|_{L^\infty(\mathbb{R}^{2d})} \left\| \Theta^x(q,p) - \Theta^x_0 \right\| & \text{if } |\beta| = 2 \\ 0 & \text{if } |\beta| \geq 3 \end{cases}
\end{aligned}$$

and a similar estimate for the y-derivatives. As

$$e^{-\frac{1}{2}} = \left\| x e^{-x^2/2} \right\|_{L^\infty(\mathbb{R}^d)} \leq \left\| x e^{-x^2/2} \right\|_{L^\infty(\mathbb{R}^d)} = 1,$$

we have

$$\left\| \partial^\alpha_{(x,y)} w(x,y,q,p) \right\| \leq C_\alpha \left\langle \left\| \Theta^x(q,p) - \Theta^x_0 \right\| \right\rangle^{|\alpha|} \left\langle \left\| \Theta^y(q,p) - \Theta^y_0 \right\| \right\rangle^{|\alpha|}$$

and so $w \in S[0,4d]$ and $v^\varepsilon \in S^{1/2}[m;4d]$ by similar arguments for the q and p derivatives. Moreover, we have

$$\partial^\alpha_{(x,y)} v^\varepsilon = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \varepsilon^{-\frac{|\beta|}{2}} \left[\partial^\beta_{(x,y)} w\right] \left(\varepsilon^{-\frac{1}{2}}(x - X^\kappa(q,p)), \varepsilon^{-\frac{1}{2}}(y-q), q, p\right) \left[\partial^{\alpha-\beta}_{(x,y)} u\right]. \tag{4.21}$$

Hence, if $u \in S[0;4d]$

$$\begin{aligned}
\sum_{|\alpha| \leq 4d+1} \varepsilon^{\frac{|\alpha|}{2}} \left\| \partial^\alpha_{(x,y)} v^\varepsilon \right\|_{L^\infty(\mathbb{R}^{4d})} &= \sum_{|\alpha| \leq 4d+1} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \varepsilon^{\frac{|\alpha|-|\beta|}{2}} \left\| \partial^\beta_{(x,y)} w \right\| \left\| \partial^{\alpha-\beta}_{(x,y)} u \right\| \\
&\leq C[\Theta^x, \Theta^y] \sum_{|\alpha| \leq 4d+1} \varepsilon^{\frac{|\alpha|}{2}} \left\| \partial^\alpha_{(x,y)} u \right\|_{L^\infty(\mathbb{R}^{4d})},
\end{aligned}$$

where

$$C[\Theta^x, \Theta^y]) = C \left\langle \left\| \Theta^x - \Theta^x_0 \right\| \right\rangle^{|\alpha|} \left\langle \left\| \Theta^y - \Theta^y_0 \right\| \right\rangle^{|\alpha|}.$$

The identity of the second point is clear. □

4.4.2 Proof of the continuity on $\mathcal{S}(\mathbb{R}^d)$

In this section we present the proof of the Schwartz-continuity result Proposition 4.10. By Lemma 4.14 it is enough to prove the result for $\varepsilon = 1$. We recall that for the continuity of $\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)$ on $\mathcal{S}(\mathbb{R}^d)$, we have to show the smoothness of $(\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi)(x)$ with respect to x and to estimate all seminorms

$$\left\|\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right\|_{\alpha,\beta} = \sup_{x\in\mathbb{R}^d}\left|x^\alpha\partial_x^\beta\left(\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right)(x)\right|$$

of this expression by a finite linear combination of $\|\varphi\|_{\alpha',\beta'}$, i.e.

$$\left\|\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right\|_{\alpha,\beta} \le C_{\alpha\beta}\sum\|\varphi\|_{\alpha'\beta'} \tag{4.22}$$

where the sum is finite and $C_{\alpha\beta}$ independent of φ.

We use two distinct methods to control growth in the variables x, q and p. First, the Gaussian decay in $x - X^\kappa(q,p)$ compensates for any polynomial growth in $x - X^\kappa(q,p)$. Thus, by the reexpansion of a polynomial in x around $X^\kappa(q,p)$, growth in x can be converted to growth in $X^\kappa(q,p)$, i.e. growth in q and p. The same idea can be used to convert growth in q to growth in y. Finally, integration by parts in y are used to convert growth in the momentum variable p into derivatives of φ.

Proof of Proposition 4.10.

Let m be a non-negative integer such that $u \in S[(2m, 2m, 2m); (d, d, 2d)]$. By Lemma 4.9 we have

$$\begin{aligned}
&\partial_x^\beta\left[(2\pi)^{3d/2}\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right](x)\\
&= \partial_x^\beta \lim_{\lambda\to\infty}\int_{\mathbb{R}^{3d}} e^{i\Phi(x,y,q,p;\Theta_0^x,\Theta_0^y)}u_\sigma^\lambda(x,y,q,p)\varphi(y)\,dq\,dp\,dy\\
&= \lim_{\lambda\to\infty}\int_{\mathbb{R}^{3d}} e^{i\Phi}\sum_{\gamma_0+\gamma=\beta}\binom{\beta}{\gamma}\sum_{k=1}^{|\gamma|} i^k \sum_{\substack{\gamma_1+\ldots+\gamma_k=\gamma\\ |\gamma_j|\ge 1}}\left(\partial_x^{\gamma_0}u_\sigma^\lambda\right)\prod_{j=1}^k\left(\partial_x^{\gamma_j}\Phi^\kappa\right)\varphi(y)\,dq\,dp\,dy
\end{aligned}$$

for $|\beta| \ge 1$. As

$$\partial_x\Phi^\kappa(x,y,q,p;\Theta_0^x,\Theta_0^y) = \Xi^\kappa(q,p) + i\Theta_0^x(x - X^\kappa(q,p)),$$

$\prod_{j=1}^k\left(\partial_x^{\gamma_j}\Phi^\kappa\right)$ is polynomial of degree at most k in $(x - X^\kappa(q,p), \Xi^\kappa(q,p))$. Recalling that κ is Lipschitz-continuous, we see that

$$\prod_{j=1}^k\left(\partial_x^{\gamma_0}u\right)\left(\partial_x^{\gamma_j}\Phi^\kappa\right) \in S[(2m + |\beta|, 2m, 2m + |\beta|); (d, d, 2d)],$$

so Lemma 4.9 shows that

$$\partial_x^\beta\left[\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right](x) = \left[\sum_{\gamma_0+\gamma=\beta}\binom{\beta}{\gamma}\sum_{k=1}^{|\gamma|} i^k\mathcal{I}^1\left(\kappa; (\partial_x^{\gamma_0}u)\prod_{j=1}^k\left(\partial_x^{\gamma_j}\Phi^\kappa\right); \Theta_0^x, \Theta_0^y\right)\varphi\right](x).$$

The smoothness of $\mathcal{I}^\varepsilon(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi$ with respect to x is a consequence of the local uniformness of the λ-limit.

We see that it is sufficient to estimate

$$\left\| \mathcal{I}^1 \left(\kappa; x^\alpha \left(\partial_x^{\gamma_0} u\right) \prod_{j=1}^{k} \left(\partial_x^{\gamma_j} \Phi^\kappa\right); \Theta_0^x, \Theta_0^y \right) \varphi \right\|_{L^\infty(\mathbb{R}^d)} .$$

Using an exact Taylor expansion in x of the polynomial $\left(\langle x \rangle^{2m} x^\alpha\right) \prod_{j=1}^{k} \left(\partial_x^{\gamma_j} \Phi^\kappa\right)$ around $X^\kappa(q,p)$ and dropping the arguments of $X^\kappa(q,p)$ and $\Xi^\kappa(q,p)$ for better readability, we get the identity

$$\frac{\langle x \rangle^{2m} x^\alpha}{\langle x \rangle^{2m}} \left(\partial_x^{\gamma_0} u_\sigma^\lambda\right) \prod_{j=1}^{k} \left(\partial_x^{\gamma_j} \Phi^\kappa\right) = \sum_{|\delta| \le |\alpha|+2m+k} P^{\alpha\delta m}_{\gamma_1,\dots,\gamma_k}[\Theta_0^x, \Theta_0^y](X^\kappa, \Xi^\kappa) \quad (x - X^\kappa)^\delta$$
$$\frac{\partial_x^{\gamma_0} u_\sigma^\lambda}{\langle x \rangle^{2m} \langle (q,p) \rangle^{2m}} \frac{\langle (q,p) \rangle^{|\alpha|+k+4m-|\delta|+2d+1+\rho_{\alpha k \delta}}}{\langle (q,p) \rangle^{|\alpha|+k+2m-|\delta|+\rho_{\alpha k \delta}} \langle (q,p) \rangle^{2d+1}},$$

where $P^{\alpha\delta m}_{\gamma_1,\dots,\gamma_k}$ is polynomial in its arguments of degree $|\alpha| + k + 2m - |\delta|$ and $\rho_{\alpha k \delta}$ is either 0 or 1 and chosen such that $|\alpha| + k - |\delta| + 1 + \rho_{\alpha k \delta}$ is even.

Now

$$\nabla_y \Phi^\kappa = p + i\Theta_0^y (y - q)$$

and thus we have

$$\begin{aligned}
&(2\pi)^{3d/2} \mathcal{I}^1(\kappa; p_j v; \Theta_0^x, \Theta_0^y)\, \psi(x) \\
&= \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} e^{i\Phi^\kappa} p_j v(x,y,q,p) \sigma(q/\lambda, p/\lambda) \varphi(y)\; dq\, dp\, dy \\
&= i \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} e^{i\Phi^\kappa} \sigma(q/\lambda, p/\lambda) \partial_{y_j} \left(v(x,y,q,p) \varphi(y) \right)\; dq\, dp\, dy \\
&\quad - i \lim_{\lambda\to\infty} \int_{\mathbb{R}^{3d}} e^{i\Phi^\kappa} \left(\Theta_0^y (y-q)\right)_j v(x,y,q,p) \sigma(q/\lambda, p/\lambda) \varphi(y)\; dq\, dp\, dy
\end{aligned}$$

for any symbol $v \in S[+\infty; 4d]$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$.

Thus using Taylor-expansion of the polynomial $\langle (q,p) \rangle^{|\alpha|+k+4m-|\delta|+2d+1+\rho_{\alpha k \delta}}$ around $q = y$ followed by integrations by parts in y we have

$$\mathcal{I}^1 \left(\kappa; x^\alpha \left(\partial_x^{\gamma_0} u\right) \prod_{j=1}^{k} \left(\partial_x^{\gamma_j} \Phi^\kappa\right); \Theta_0^x, \Theta_0^y \right) \varphi = \sum_{\substack{|\delta| \le |\alpha|+2m+k \\ \mu_0+\mu_1 \le |\alpha|+k+4m-|\delta|+2d+1+\rho_{\alpha k \delta} \\ |\delta'| \le |\alpha|+k+4m+2d+1-|\delta|+\rho_{\alpha k \delta}+|\mu_0|+|\mu_1|}}$$
$$\mathcal{I}^1 \left(\kappa; \frac{P^{\alpha\delta m}_{\gamma_1,\dots,\gamma_k}[\Theta_0^x, \Theta_0^y](X^\kappa, \Xi^\kappa)}{\langle (q,p) \rangle^{|\alpha|+k+2m-|\delta|+\rho_{\alpha k \delta}+2d+1} \langle y \rangle^{d+1}} \frac{(x - X^\kappa)^\delta (\partial_x^{\gamma_0} \partial_y^{\mu_0} u)}{(\langle y \rangle \langle x \rangle \langle (q,p) \rangle)^{2m}} (q-y)^{\delta'}; \Theta_0^x, \Theta_0^y \right)$$
$$\left[\langle y \rangle^{2m+d+1} Q^{\alpha k m \delta \rho_{\alpha k \delta} \mu_0 \mu_1 \delta'}_{\gamma_1,\dots,\gamma_k}[\Theta_0^y](y) \partial_y^{\mu_1} \varphi \right] \tag{4.23}$$

where $Q^{\alpha k m \delta \rho_{\alpha k \delta} \mu_0 \mu_1 \delta'}_{\gamma_1,\dots,\gamma_k}[\Theta_0^y]$ is polynomial of degree $|\alpha| + k + 4m - |\delta| + 2d + 1 + \rho_{\alpha k \delta}$ with coefficients depending on Θ_0^y.

We have now established all necessary decay to prove a sufficient upper bound on the former expression. As κ is Lipschitz-continuous and the degree of $P^{\alpha\delta m}_{\gamma_1,\dots,\gamma_k}[\Theta^x_0,\Theta^y_0]$ is $|\alpha|+k+2m-|\delta|$, we have

$$\left\|\frac{P^{\alpha\delta m}_{\gamma_1,\dots,\gamma_k}[\Theta^x_0,\Theta^y_0](X^\kappa(q,p),\Xi^\kappa(q,p))}{\langle(q,p)\rangle^{|\alpha|+k+2m-|\delta|}}\right\|_{L^\infty(\mathbb{R}^{2d})}\le C^{\alpha\delta mk}_{\gamma_1,\dots,\gamma_k}[\Theta^x_0,\Theta^y_0].$$

Moreover

$$\left\|(q-y)^{\delta'}e^{-\Theta^y_0(q-y)^2/2}\right\|_{L^\infty(\mathbb{R}^{2d})}\le C^{\delta'}[\Theta^y_0]\quad\text{and}$$
$$\left\|(x-X^\kappa)^{\delta}e^{-\Theta^x_0(x-X^\kappa)^2/2}\right\|_{L^\infty(\mathbb{R}^{3d})}\le C^{\delta}[\Theta^x_0].$$

Thus every term in the sum on the right-hand side in (4.23) is dominated by

$$C^{\alpha\delta mk}_{\gamma_1,\dots,\gamma_k}[\Theta^x_0,\Theta^y_0]C^{\delta'}[\Theta^y_0]C^{\delta}[\Theta^x_0]\left\|\langle(q,p)\rangle^{-(2d+1)}\right\|_{L^1(\mathbb{R}^{2d})}\left\|\langle y\rangle^{-(d+1)}\right\|_{L^1(\mathbb{R}^{d})}$$
$$\times\left\|\frac{\partial_x^{\gamma_0}\partial_y^{\mu_0}u}{(\langle y\rangle\langle x\rangle\langle(q,p)\rangle)^{2m}}\right\|_{L^\infty(\mathbb{R}^{4d})}\sum_{|\alpha'|\le|\alpha|+k+6m-|\delta|+3d+2+\rho_{\alpha k\delta}}\left\|\langle y\rangle^{\alpha'}\partial_y^{\mu_1}\varphi\right\|_{L^\infty(\mathbb{R}^{d})}$$

and, noting that

$$\|\langle y\rangle^{\alpha}\psi\|_{L^\infty(\mathbb{R}^d)}\le C\left[\|\psi\|_{L^\infty(\mathbb{R}^d)}+\sum_{|\beta|=|\alpha|}\left\|y^\beta\psi\right\|_{L^\infty(\mathbb{R}^d)}\right],$$

we have established the bound

$$\begin{aligned}&\left\|\mathcal{I}^1(\kappa;u;\Theta^x_0,\Theta^y_0)\,\varphi\right\|_{\alpha\beta}\\&\le C_{\alpha\beta}[\Theta^x_0,\Theta^y_0]\sum_{|\alpha'|\le|\alpha|+2|\beta|+4m+2d+2}\left\|\frac{\partial^{\alpha'}_{(x,y)}u}{(\langle x\rangle\langle y\rangle\langle(q,p)\rangle)^{2m}}\right\|_{L^\infty(\mathbb{R}^{4d})}\sum_{\substack{|\alpha'|\le|\alpha|+|\beta|+6m+3d+3\\|\beta'|\le|\alpha|+|\beta|+4m+2d+2}}\|\varphi\|_{\alpha'\beta'},\end{aligned}\tag{4.24}$$

which proves the result. □

4.4.3 Proof of the continuity on $L^2(\mathbb{R}^d)$

As the Calderón-Vaillancourt Theorem, the proof of the L^2-boundedness is based on the Cotlar-Stein Lemma, see Lemma 2.8.3 in [Mar02].

4.16 Lemma (Cotlar-Stein). *Let $(\mathcal{I}_\Gamma)_{\Gamma\in\mathbb{Z}^n}$ a family of bounded operators on $L^2(\mathbb{R}^d)$ satisfying*

$$\forall\Gamma,\Gamma'\in\mathbb{Z}^n,\quad\|\mathcal{I}^*_\Gamma\mathcal{I}_{\Gamma'}\|_{L^2\to L^2}+\|\mathcal{I}_\Gamma\mathcal{I}^*_{\Gamma'}\|_{L^2\to L^2}\le\omega(\Gamma-\Gamma')\tag{4.25}$$

and

$$\sum_{\Gamma\in\mathbb{Z}^n}\sqrt{\omega(\Gamma)}<\infty.$$

Then the series $\sum_{\Gamma\in\mathbb{Z}^n}\mathcal{I}_\Gamma$ is strongly convergent to a bounded operator $\mathcal{I}_\infty$ with

$$\|\mathcal{I}_\infty\|_{L^2\to L^2}\le\sum_{\Gamma\in\mathbb{Z}^d}\sqrt{\omega(\Gamma)}.$$

This lemma is used in the following way: first, one uses a partition of unity to represent the symbol u as a series over symbols u_Γ, which are compactly supported in (q,p) for sets K_Γ, i.e.

$$u(x,y,q,p) = \sum_{\Gamma \in \mathbb{Z}^d} u_\Gamma(x,y,q,p);$$

in a second step, one establishes bounds of the form (4.25), which decay in the distance of the supports of the u_Γ and shows that the strong limit provided by Lemma 4.16 coincides with $\mathcal{I}^1(\kappa; u; \Theta^x, \Theta^y)$.

Formal adjoints

Due to the high symmetry of the phase function Φ^κ, it is enough to treat either the operator $\mathcal{I}_\Gamma^* \mathcal{I}_{\Gamma'}$ or $\mathcal{I}_\Gamma \mathcal{I}_{\Gamma'}^*$.

4.17 Definition. *Let $\mathcal{I}, \mathcal{I}^{(*)} : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d)$ be two linear operators. We say that $\mathcal{I}^{(*)}$ is a* **formal adjoint** *of $\mathcal{I}$ if*

$$\langle \mathcal{I}\varphi | \psi \rangle_{L^2(\mathbb{R}^d)} = \left\langle \varphi \middle| \mathcal{I}^{(*)} \psi \right\rangle_{L^2(\mathbb{R}^d)}$$

for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}^d)$.

If it exists, a formal adjoint is necessarily unique because of the density of $\mathcal{S}(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$. For bounded operators, a formal adjoint coincides with the adjoint of the operator due to the density of $\mathcal{S}(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$. For our FIOs, we have

4.18 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[+\infty; 4d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$. Then $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ has a formal adjoint which is given by*

$$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)^{(*)} = e^{\frac{i}{\varepsilon}C} \mathcal{I}^\varepsilon\left(\kappa^{-1}; u^\kappa; \Theta^{y,\kappa}, \Theta^{x,\kappa}\right),$$

where

$$u^\kappa(x,y,q,p) = \overline{u(y,x,X^{\kappa^{-1}}(q,p), \Xi^{\kappa^{-1}}(q,p))}$$
$$\Theta^{x,\kappa} = \overline{\Theta^x \circ \kappa^{-1}}, \quad \Theta^{y,\kappa} = \overline{\Theta^y \circ \kappa^{-1}}.$$

and C is a constant depending on the actions associated to κ and κ^{-1}.

Proof. Let $\varphi, \psi \in \mathcal{S}(\mathbb{R}^d)$. We have

$$\begin{aligned}
&(2\pi\varepsilon)^{3d/2} \left\langle \mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\, \varphi | \psi \right\rangle_{L^2(\mathbb{R}^d)} \\
&= \lim_{\lambda\to\infty} \int_{\mathbb{R}^d} \left[\int_{\mathbb{R}^{3d}} \sigma(q/\lambda, p/\lambda) e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)} u(x,y,q,p)\varphi(y)\, dq\, dp\, dy \right] \overline{\psi(x)}\, dx \\
&= \lim_{\lambda\to\infty} \int_{\mathbb{R}^{4d}} \varphi(y) \overline{\left[e^{-\frac{i}{\varepsilon}\overline{\Phi^\kappa(x,y,q,p;\Theta^x,\Theta^y)}} \overline{u_\sigma^\lambda(x,y,q,p)} \psi(x) \right]}\, dq\, dp\, dx\, dy,
\end{aligned}$$

where we used dominated convergence for the exchange of the limit and the integration. We perform the symplectic change of variables $(q,p) \mapsto \kappa(q,p)$ and obtain

$$\begin{aligned}
&- \overline{\Phi^\kappa\left(x, y, X^{\kappa^{-1}}(q,p), \Xi^{\kappa^{-1}}(q,p); \Theta^x, \Theta^y\right)} \\
&= -\left(S^\kappa \circ \kappa^{-1}\right)(q,p) + \Xi^{\kappa^{-1}}(q,p) \cdot \Big(y - X^{\kappa^{-1}}(q,p)\Big) \\
&\quad - p\cdot(x-q) + i\overline{\left(\Theta^x \circ \kappa^{-1}\right)(q,p)}(x-q)^2/2 + i\overline{\left(\Theta^y \circ \kappa^{-1}\right)(q,p)}(y - X^{\kappa^{-1}}(q,p))^2/2 \\
&= C + \Phi^{\kappa^{-1}}\left(y, x, q, p; \Theta^{y,\kappa}, \Theta^{x,\kappa}\right),
\end{aligned}$$

where we used Proposition 2.5 for the expression of the action. Thus

$$
\begin{aligned}
&(2\pi\varepsilon)^{3d/2}\left\langle \mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi|\psi\right\rangle_{L^2(\mathbb{R}^d)}\\
&=\lim_{\lambda\to\infty}\int_{\mathbb{R}^{4d}}\varphi(y)\overline{\left[e^{\frac{i}{\varepsilon}C}e^{\frac{i}{\varepsilon}\Phi^{\kappa^{-1}}(x,y,q,p;\overline{\Theta^{y,\kappa}},\overline{\Theta^{x,\kappa}})}u^\kappa(y,x,q,p)\sigma(\kappa^{-1}(q,p)/\lambda)\psi(x)\right]}\,dq\,dp\,dx\,dy\\
&=\lim_{\lambda\to\infty}\int_{\mathbb{R}^{4d}}\sigma(\kappa^{-1}(q,p)/\lambda)\varphi(y)\overline{\left[e^{\frac{i}{\varepsilon}C}e^{\frac{i}{\varepsilon}\Phi^{\kappa^{-1}}}u^\kappa(y,x,q,p)\psi(x)\,dq\,dp\,dx\right]}\,dy\\
&=(2\pi\varepsilon)^{3d/2}\left\langle\varphi\middle|e^{\frac{i}{\varepsilon}C}\mathcal{I}^\varepsilon\left(\kappa^{-1};u^\kappa;\Theta^{x,\kappa},\Theta^{y,\kappa}\right)\psi\right\rangle_{L^2(\mathbb{R}^d)},
\end{aligned}
$$

by dominated convergence. □

We will use the following corollary.

4.19 Corollary. *Let κ_1,κ_2 be canonical transformations of class $\mathcal{B}$, $u_1,u_2\in S[+\infty;4d]$ and $\Theta_0^x,\Theta_0^y\in\mathcal{C}_{\text{const}}$. Then*

$$
\begin{aligned}
\mathcal{I}^\varepsilon(\kappa_1;u_1;\Theta_0^x,\Theta_0^y)\,&\mathcal{I}^\varepsilon(\kappa_2;u_2;\Theta_0^x,\Theta_0^y)^{(*)}\\
&=e^{\frac{i}{\varepsilon}C}\mathcal{I}^\varepsilon\left(\kappa_1^{-1};u_1^{\kappa_1};\Theta_0^y,\Theta_0^x\right)^{(*)}\mathcal{I}^\varepsilon\left(\kappa_2^{-1};u_2^{\kappa_2};\Theta_0^y,\Theta_0^x\right),
\end{aligned}
$$

where C depends on the actions associated to $\kappa_1,\kappa_2,\kappa_1^{-1}$ and κ_2^{-1}.

Estimate on FIOs with compactly supported symbols

The estimates (4.25) on the operators $\mathcal{I}_\Gamma\mathcal{I}_{\Gamma'}^*$ will be established with help of a classical Lemma of Schur, Lemma 2.8.4 in [Mar02].

4.20 Lemma (Schur)**.** *If $A\varphi(x)=\int_{\mathbb{R}^d}K(x,y)\varphi(y)\,dy$ with $K\in C(\mathbb{R}^d\times\mathbb{R}^d;\mathbb{C})$, then*

$$
\|A\|_{L^2\to L^2}\le\left(\sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}|K(x,y)|\;dy\right)^{1/2}\left(\sup_{y\in\mathbb{R}^d}\int_{\mathbb{R}^d}|K(x,y)|\;dx\right)^{1/2}.
$$

In a first step, we will establish an estimate on the composition of FIOs with compact support. We recall that the Hausdorf distance of two sets $K_1,K_2\subset\mathbb{R}^{2d}$ is given by

$$
\delta\left(K_1,K_2\right)=\min_{(q_j,p_j)\in K_j}|(q_1,p_1)-(q_2,p_2)|
$$

and introduce the additional notation

$$
\delta_\kappa\left(K_1,K_2\right)=\delta\left(\kappa(K_1),\kappa(K_2)\right)=\min_{(q_j,p_j)\in K_j}|\kappa(q_1,p_1)-\kappa(q_2,p_2)|
$$

for the κ-deformed Haussdorff-distance of two sets and recall that the linear canonical transformation $\Lambda[\Theta]$ is given by

$$
\Lambda[\Theta](q,p)=\begin{pmatrix}(\Theta)^{1/2}&\\&(\Theta)^{-1/2}\end{pmatrix}\begin{pmatrix}q\\p\end{pmatrix}.
$$

4.21 Proposition. *Let κ be a canonical transformation of class $\mathcal{B}$, $\Theta_0^x, \Theta_0^y \in \mathcal{C}_{\text{const}}$ and $u, v \in S[(0,-\infty);(2d,2d)]$ be compactly supported in (q,p) independently of x and y, i.e.* $\operatorname{supp}(u) \subset \mathbb{R}^{2d} \times K_u$ *and* $\operatorname{supp}(v) \subset \mathbb{R}^{2d} \times K_v$*, where K_u and K_v are compact subsets of $\mathbb{R}^{2d}$. Then, for any $l \in \mathbb{N}$,*

$$\left\|\mathcal{I}^1(\kappa; v; \Theta_0^x, \Theta_0^y)\, \mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)^*\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C_l \frac{\sum_{|\alpha|+|\beta|\le l} (\lambda^y)^{-\frac{|\alpha|+|\beta|}{2}} \left\|\partial_y^\alpha u\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}} \left\|\partial_y^\beta v\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}}}{(\det \Theta_0^x \det \Theta_0^y)^{1/2} \left(1 + \delta^2_{\Lambda[\Theta_0^y]}\left[K_u, K_v\right]\right)^{l/2}} \tag{4.26}$$

$$\left\|\mathcal{I}^1(\kappa; v; \Theta_0^x, \Theta_0^y)^*\, \mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C_l \frac{\sum_{|\alpha|+|\beta|\le l} (\lambda^x)^{-\frac{|\alpha|+|\beta|}{2}} \left\|\partial_x^\alpha u\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}} \left\|\partial_x^\beta v\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}}}{(\det \Theta_0^x \det \Theta_0^y)^{1/2} \left(1 + \delta^2_{\Lambda[\Theta_0^x]\circ\kappa}\left[K_u, K_v\right]\right)^{l/2}}. \tag{4.27}$$

We want to recall that the assumption Θ_0^x, Θ_0^y means in particular, that Θ_0^x and Θ_0^y are real matrices. In principle, it is possible to prove the result for complex symmetric positive definite matrices Θ_0^x and Θ_0^y, compare the corresponding result in [RS08]. However, due to Lemma 4.15 it is sufficient to treat the simpler case here.

Proof. We have

$$(2\pi)^{3d}\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\, \mathcal{I}^1(\kappa; v; \Theta_0^x, \Theta_0^y)^*\, \varphi(x) = \int_{\mathbb{R}^d} K(x,y)\varphi(y)\, dy,$$

where the integral kernel $K(x,y)$ is given by the absolutely convergent integral

$$\int_{\mathbb{R}^{5d}} e^{i\Omega^\kappa(x,y,w,q_1,q_2,p_1,p_2;\Theta_0^x,\Theta_0^y)} u(x,w,q_1,p_1)\overline{v(y,w,q_2,p_2)}\, dq_1\, dq_2\, dp_1\, dp_2\, dw$$

with phase function

$$\begin{aligned}
&\Omega^\kappa(x,y,w,q_1,q_2,p_1,p_2;\Theta_0^x,\Theta_0^y)\\
&= \Phi^\kappa(x,w,q_1,p_1;\Theta_0^x,\Theta_0^y) - \overline{\Phi^\kappa(y,w,q_2,p_2;\Theta_0^x,\Theta_0^y)}\\
&= S^\kappa(q_1,p_1) - S^\kappa(q_2,p_2) - p_1\cdot(w-q_1) + p_2\cdot(w-q_2)\\
&\quad + \Xi^\kappa(q_1,p_1)\cdot(x - X^\kappa(q_1,p_1)) - \Xi^\kappa(q_2,p_2)\cdot(y - X^\kappa(q_2,p_2))\\
&\quad + i\Theta_0^x\left(x - X^\kappa(q_1,p_1)\right)^2/2 + i\Theta_0^x\left(y - X^\kappa(q_2,p_2)\right)^2/2\\
&\quad + i\Theta_0^y\left(w-q_1\right)^2/2 + i\Theta_0^y\left(w-q_2\right)^2/2.
\end{aligned}$$

Hence

$$\begin{aligned}
\Im\Omega^\kappa &= \Theta_0^x(x - X^\kappa(q_1,p_1))^2/2 + \Theta_0^x(y - X^\kappa(q_2,p_2)^2/2\\
&\quad + \Theta_0^y\left(w - \frac{q_1+q_2}{2}\right)^2 + \Theta_0^y\left(\frac{q_1-q_2}{2}\right)^2
\end{aligned}$$

and

$$\nabla_w \Omega^\kappa = (p_2 - p_1) + 2i\Theta_0^y \left(w - \frac{q_1 + q_2}{2} \right).$$

We introduce the first order differential operator

$$L_w = \frac{1 - i \left(\Theta_0^y\right)^{-1} \overline{\nabla_w \Omega^\kappa} \cdot \nabla_w}{1 + \left| \left(\Theta_0^y\right)^{-1/2} \nabla_w \Omega^\kappa \right|^2},$$

which fulfills $L_w e^{i\Omega^\kappa} = e^{i\Omega^\kappa}$ and

$$\left| \left(L_w^\dagger \right)^l (u\overline{v}) \right| \leq \frac{M_l^w}{\left\langle \left(\Theta_0^y\right)^{-1/2} \nabla_w \Omega^\kappa \right\rangle^l} \sum_{|\alpha| \leq l} \left| \left(\left(\Theta_0^y\right)^{-1/2} \nabla_w \right)^\alpha (u\overline{v}) \right|,$$

compare Lemma 10.2. Hence we have

$$\begin{aligned}
&|K(x,y)| \\
&= \left| \int_{\mathbb{R}^{5d}} e^{i\Omega^\kappa} \left(L_w^\dagger \right)^l \left[u(x,w,q_1,p_1) \overline{v(y,w,q_2,p_2)} \right] \, dq_1 \, dq_2 \, dp_1 \, dp_2 \, dw \right| \\
&\leq M_l^w \int_{\mathbb{R}^{5d}} e^{-\Theta_0^x (x - X^\kappa(q_1,p_1))^2/2} e^{-\Theta_0^x (y - X^\kappa(q_2,p_2))^2/2} e^{-\Theta_0^y (q_1 - q_2)^2/4} e^{-\Theta_0^y \left(w - \frac{q_1+q_2}{2} \right)^2} \\
&\qquad \left\langle \left(\Theta_0^y\right)^{-1/2} (p_1 - p_2) \right\rangle^{-l} \left\langle \left(\Theta_0^y\right)^{1/2} (q_1 - q_2) \right\rangle^{-l} \left\langle \left(\Theta_0^y\right)^{1/2} (q_1 - q_2) \right\rangle^{l} \\
&\qquad \sum_{|\alpha| \leq l} (\lambda^y)^{-\frac{|\alpha|}{2}} \left| \partial_w^\alpha \left[u(x,w,q_1,p_1) \overline{v(y,w,q_2,p_2)} \right] \right| \, dq_1 \, dp_1 \, dq_2 \, dp_2 \, dw
\end{aligned} \tag{4.28}$$

and we can estimate

$$\begin{aligned}
&\sup_{x \in \mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y)| \, dy \\
&\leq M_l^w \left\| e^{-q^2/4} \langle q \rangle^l \right\|_{L^\infty(\mathbb{R}^d)} \left\| e^{-\Theta_0^x y^2/2} \right\|_{L^1(\mathbb{R}^d)} \left\| e^{-\Theta_0^y w^2/2} \right\|_{L^1(\mathbb{R}^d)} \left\langle \delta_{\Lambda[\Theta_0^y]}(K_u, K_v) \right\rangle^{-l} \\
&\qquad \sup_{(x,y,w) \in \mathbb{R}^{3d}} \int_{\mathbb{R}^{4d}} \sum_{|\alpha| \leq l} (\lambda^y)^{-\frac{|\alpha|}{2}} \left| \partial_w^\alpha (u(x,w,q_1,p_1) \overline{v(y,w,q_2,p_2)} \right| \, dq_1 \, dp_1 \, dq_2 \, dp_2 \\
&\leq C_l \det \left(\Theta_0^x \Theta_0^y\right)^{1/2} \sum_{|\alpha| + |\beta| \leq l} (\lambda^y)^{-\frac{|\alpha|+|\beta|}{2}} \left\langle \delta_{\Lambda[\Theta_0^y]}(K_u, K_v) \right\rangle^{-l} \left\| \partial_y^\alpha u \right\|_{L^\infty_{(x,y)} L^1_{(q,p)}} \left\| \partial_y^\beta v \right\|_{L^\infty_{(x,y)} L^1_{(q,p)}}.
\end{aligned}$$

As (4.28) is symmetric in x and y, we get exactly the same estimate for

$$\sup_{y \in \mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y)| \, dx$$

and the Schur Lemma yields (4.26).

Using Corollary 4.19 and the fact that

$$\operatorname{supp}(u^\kappa) \subset \mathbb{R}^{2d} \times \kappa(K_u), \qquad \operatorname{supp}(v^\kappa) \subset \mathbb{R}^{2d} \times \kappa(K_v),$$

(4.26) translates into

$$\begin{aligned}
&\left\|\mathcal{I}^1(\kappa; v; \Theta_0^x, \Theta_0^y)^* \mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \\
&\quad \le C_l \frac{\sum_{|\alpha|+|\beta|\le l} (\lambda^x)^{-\frac{|\alpha|+|\beta|}{2}} \left\|\partial_y^\alpha u^\kappa\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}} \left\|\partial_y^\beta v^\kappa\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}}}{(\det \Theta_0^x \det \Theta_0^y)^{1/2} \left(1 + \delta^2_{\Lambda[\Theta_0^x]}\left[\kappa(K_u), \kappa(K_v)\right]\right)^{l/2}} \\
&\quad = C_l \frac{\sum_{|\alpha|+|\beta|\le l} (\lambda^x)^{-\frac{|\alpha|+|\beta|}{2}} \left\|\partial_x^\alpha u\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}} \left\|\partial_x^\beta v\right\|_{L^\infty_{(x,y)} L^1_{(q,p)}}}{(\det \Theta_0^x \det \Theta_0^y)^{1/2} \left(1 + \delta^2_{\Lambda[\Theta_0^x]\circ\kappa}\left[K_u, K_v\right]\right)^{l/2}},
\end{aligned}$$

which is (4.27). □

Proof of Theorem 4.11

Proof of Theorem 4.11. By Lemmas 4.14 and 4.15, it is enough to prove the result for $\varepsilon = 1$ and $\Theta_0^x, \Theta_0^y \in \mathcal{C}_{\text{const}}$. We introduce a partition of unity of the phase-space in the following way. We choose a function $\chi \in C_0^\infty(\mathbb{R}^{2d}; [0,1])$ with

$$\begin{aligned}
\operatorname{supp}\chi &\subset \left[-\frac{3}{4}, \frac{3}{4}\right]^{2d} =: K \\
\chi(z) = 1 &\quad \text{for} \quad z \in \left[-\frac{1}{4}, \frac{1}{4}\right]^{2d} \quad \text{and} \\
\sum_{\Gamma\in\mathbb{Z}^{2d}} \chi_\Gamma = 1, &\quad \text{where } \chi_\Gamma(z) := \chi(z - \Gamma),
\end{aligned}$$

compare Figure 4.1.

In the second step, we define the symbols u_Γ by $u_\Gamma(x,y,q,p) := \chi_\Gamma(q,p)u(x,y,q,p)$, which are supported in $\mathbb{R}^{2d} \times [K+\Gamma]$. Noting that the size of K is smaller than $\left(1+\frac{1}{2}\right)^{4d}$, Proposition 4.21 shows that

$$\left\|\mathcal{I}^1(\kappa; u_{\Gamma_1}; \Theta_0^x, \Theta_0^y)\, \mathcal{I}^1(\kappa; u_{\Gamma_2}; \Theta_0^x, \Theta_0^y)^*\right\| + \left\|\mathcal{I}^1(\kappa; u_{\Gamma_1}; \Theta_0^x, \Theta_0^y)^*\, \mathcal{I}^1(\kappa; u_{\Gamma_2}; \Theta_0^x, \Theta_0^y)\right\|$$

is dominated by

$$\begin{aligned}
&\omega(\Gamma_1 - \Gamma_2) \\
&:= \frac{C_l \min(1, \lambda^x, \lambda^y)^{-l/2} (1+2\nu)^{4d}}{(\det \Theta_0^x \det \Theta_0^y)^{1/2} \left(1 + \eta^2_{[\kappa;\Theta_0^x,\Theta_0^y]} \delta^2(\operatorname{supp}(u_{\Gamma_1}), \operatorname{supp}(u_{\Gamma_2}))\right)^{l/2}} \|u\|^2_{W^{l,\infty}_{(x,y)} L^\infty_{(q,p)}},
\end{aligned}$$

where

$$\eta_{[\kappa;\Theta_0^x,\Theta^y]} = \min\left(c_{\Lambda[\Theta_0^x]\circ\kappa}, c_{\Lambda[\Theta_0^y]}\right).$$

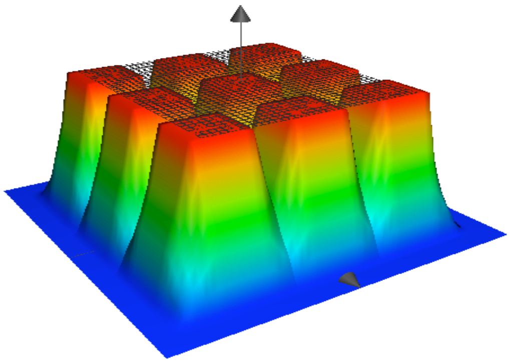

Figure 4.1: An example for a function χ and some of its translates with their sum indicated by the grey grid

If $|\Gamma_1 - \Gamma_2|_\infty \geq 2$, we have

$$\delta^2(\operatorname{supp}(u_\Gamma), \operatorname{supp}(u_{\Gamma'})) \geq |\Gamma_1 - \Gamma_2|_\infty - \left(1 + \frac{1}{2}\right) > 0.$$

As the number of Γ with $|\Gamma|_\infty \leq k$ equals $(2k+1)^{2d}$, we obtain

$$\frac{(\det \Theta_0^x \det \Theta_0^y)^{\frac{1}{4}}}{\sqrt{C_l}\min(1, \lambda^x, \lambda^y)^{-l/4}(1+2\nu)^{2d}\|u\|_{W^{l,\infty}_{(x,y)}L^\infty_{(q,p)}}} \sum_{\Gamma\in\mathbb{Z}^{2d}} \sqrt{\omega(\Gamma)}$$
$$\leq 3^{2d} + \sum_{k\geq 2} \frac{(2k+1)^{2d} - (2k-1)^{2d}}{\left(1 + \eta^2_{[\kappa;\Theta_0^x,\Theta_0^y]}[k - (1+\frac{1}{2})]^2\right)^{l/4}}$$
$$\leq 3^{2d} + C \sum_{k\geq 1} \frac{k^{2d-1}}{\left(1 + \eta^2_{[\kappa;\Theta_0^x,\Theta_0^y]} k^2/2\right)^{l/4}}.$$

To assure convergence of the series, we need

$$l/2 - (2d-1) > 1,$$

so the smallest integer l we can choose is $l = 4d+1$.

The Cotlar-Stein Lemma now shows that the series

$$\sum_\Gamma \mathcal{I}^1(\kappa; u_\Gamma; \Theta_0^x, \Theta_0^y)$$

is strongly convergent to a bounded operator whose norm is dominated by (4.15). It remains to show that this operator coincides with the Fourier Integral Operator defined before. But if

$\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\left(\sum_\Gamma \mathcal{I}^1(\kappa; u_\Gamma; \Theta_0^x, \Theta_0^y)\,\varphi\right)(x) = \sum_\Gamma \int e^{i\Phi^\kappa}\left(L_y^\dagger u_\Gamma \varphi\right)^k (x,y,q,p)\,dq\,dp\,dy$$

$$= \int e^{i\Phi^\kappa}\left[\left(L_y^\dagger\right)^k \sum_\Gamma u_\Gamma \varphi\right](x,y,q,p)\,dq\,dp = \left(\mathcal{I}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right)(x)$$

by dominated convergence. □

We close the chapter with the proof of Corollary 4.12.

Proof of Corollary 4.12.
The proof follows the idea of Lemma 4.15. We choose lower bounds Θ_0^x and Θ_0^y for Θ^x and Θ^y and set

$$w(x,y,q,p) = x^\alpha \exp\left[-\left[(\Theta^x(q,p) - \Theta_0^x)^{\frac{1}{2}}\,x\right]^2/2\right]$$
$$y^\beta \exp\left[-\left[(\Theta^y(q,p) - \Theta_0^y)^{\frac{1}{2}}\,y\right]^2/2\right].$$

Defining

$$v^\varepsilon(x,y,q,p) = u(x,y,q,p)\varepsilon^{\frac{|\alpha|+|\beta|}{2}} w\left(\varepsilon^{-\frac{1}{2}}(x - X^\kappa(q,p)), \varepsilon^{-\frac{1}{2}}(y-q), q, p\right),$$

we have

$$\mathcal{I}^\varepsilon\Big(\kappa; (x - X^\kappa(q,p))^\alpha\,(y-q)^\beta\,u; \Theta^x, \Theta^y\Big) = \mathcal{I}^\varepsilon(\kappa; v^\varepsilon; \Theta_0^x, \Theta_0^y)$$

and

$$\sum_{|\alpha'|\le 4d+1} \varepsilon^{\frac{|\alpha'|}{2}} \left\|\partial_{(x,y)}^{\alpha'} v^\varepsilon\right\|_{L^\infty(\mathbb{R}^{4d})}$$
$$= \sum_{|\alpha'|\le 4d+1}\sum_{\beta'\le\alpha'} \binom{\alpha'}{\beta'} \varepsilon^{\frac{|\alpha|+|\beta|}{2}} \varepsilon^{\frac{|\alpha'|-|\beta'|}{2}} \left\|\partial_{(x,y)}^{\beta'} w\right\| \left\|\partial_{(x,y)}^{\alpha'-\beta'} u\right\|$$
$$\le C[\Theta^x, \Theta^y]\varepsilon^{\frac{|\alpha|+|\beta|}{2}} \sum_{|\alpha'|\le 4d+1} \varepsilon^{\frac{|\alpha'|}{2}} \left\|\partial_{(x,y)}^{\alpha'} u\right\|_{L^\infty(\mathbb{R}^{4d})},$$

which yields the claimed norm bound. □

5 Towards the composition with PDOs

We take a first glimpse at the composition of PDOs and FIOs. Formally, we have

$$\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y) = (2\pi\varepsilon)^{-3d/2}\int_{\mathbb{R}^{3d}} e^{\frac{i}{\varepsilon}\Phi^\kappa} v(x,y,q,p)\varphi(y)\; dq\,dp\,dy,$$

where the symbol v is given by the oscillatory integral

$$\begin{aligned} v(x,y,q,p) &= e^{-i\Xi^\kappa\cdot(x-X^\kappa(q,p))/\varepsilon+\Theta^x(q,p)(x-X^\kappa(q,p))^2/2\varepsilon} \\ &\frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^2} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')}e^{i\Xi^\kappa\cdot(x'-X^\kappa(q,p))/\varepsilon-\Theta^x(q,p)(x'-X^\kappa)^2/2\varepsilon} h\left(\frac{x+x'}{2},\xi\right) u(x',y,q,p)\; dx'\,d\xi. \end{aligned}$$

Now the question arises, whether v^ε is in a good symbol class, that is if the exponential growth $e^{\Theta^x(q,p)(x-X^\kappa(q,p))^2/2\varepsilon}$ with respect to x' is compensated by the application of $\mathrm{op}^\varepsilon(h)$ to the Gaussian $e^{-\Theta^x(q,p)(x'-X^\kappa(q,p))^2/2\varepsilon}$. In general this is not the case. Consider $\varepsilon = d = \Theta^x = \Theta^y = 1$, $\kappa = \mathrm{id}$, $h(x,\xi) = \cos(\xi)$ and $u \in S[0;2]$. We have

$$\begin{aligned} v(x,q,p) &= \frac{1}{\sqrt{2\pi}} e^{(x-q)^2/2-ip\cdot(x-q)}\int_{\mathbb{R}} e^{i\xi\cdot x}e^{-(\xi-p)^2/2-i\xi q}\cos(\xi)\, u(q,p)\; d\xi \\ &= e^{-1/2}\cosh(q-x+ip)u(q,p) \end{aligned}$$

which is exponentially growing with repect to x and q and thus not in $S[+\infty;3]$. Hence, the composition is not covered by the L^2-boundedness result in Theorem 4.11, though the operator $\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;u;\mathrm{id},\mathrm{id})$ is bounded.

This particular example points to a more general problem: as $\mathcal{I}^\varepsilon(\mathrm{id};u;\mathrm{id},\mathrm{id})$ is the Anti-Wick quantisation of u, the symbol v^ε would be Anti-Wick symbol of the operator $\mathrm{op}^\varepsilon(h)$. Recalling the discussion at the beginning of this part, we know that this symbol can only exist if h is "de-smoothable" with a Gaussian. In particular, we can only expect the existence if h an holomorphic function of the variable $x+i\xi$ but even in this case, the symbol will in general not be covered by Theorem 4.11. To circumvent this problem, we will provide additional $\mathcal{S}$ and L^2-continuity results for more general oscillatory integral operators.

5.1 Another class of Fourier Integral Operators

The composition of a PDO and an FIO is formally given by

$$\begin{aligned} &[\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;v;\Theta^x,\Theta^y)\,\varphi]\,(x) \\ &= (2\pi\varepsilon)^{-5d/2}\int_{\mathbb{R}^{5d}} e^{\frac{i}{\varepsilon}\Psi^\kappa} h\left(\frac{x+x'}{2},\xi\right) v(x',y,q,p)\varphi(y)\; dq\,dp\,dy\,dx'\,d\xi', \end{aligned}$$

where the phase function Ψ^κ reads

$$\Psi^\kappa(x,\xi,x',y,q,p;\Theta^x,\Theta^y) := (x-x')\cdot\xi + \Phi^\kappa(x',y,q,p;\Theta^x,\Theta^y). \tag{5.1}$$

Of course the composition is continuous from $\mathcal{S}(\mathbb{R}^d)$ to itself and extends to $L^2(\mathbb{R}^d)$ as a bounded operator, if $v \in S[0;4d]$ and $h \in S[0;2d]$. However, when we will establish an asymptotic expansion of the composition, we will meet operators, whose symbols u cannot be written in the product form

$$u(x,\xi,x',y,q,p) = h\left(\frac{x+x'}{2},\xi\right) v(x',y,q,p) \tag{5.2}$$

and we will have to deal with operators, which are formally given by

$$(\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi)\,(x) := (2\pi\varepsilon)^{-5d/2} \int_{\mathbb{R}^{5d}} e^{\frac{i}{\varepsilon}\Psi^\kappa} u(x,\xi,x',y,q,p)\varphi(y)\; dq\,dp\,dx'\,d\xi'\,dy. \tag{5.3}$$

In this section we will prove results analogous to Proposition 4.10 and Theorem 4.11 for operators of the form (5.3). We start with the precise definition.

5.1 Definition (Fourier Integral Operator with complex phase)**.** *For a canonical transformation κ, a symbol $u \in S[(+\infty, m_\xi, +\infty, m_p);(d,d,3d,d)]$, $\Theta^x, \Theta^y \in \mathcal{C}$, $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $k_\xi > m_\xi + d$, $k_p > k_\xi + m_p + d$ we define*

$$(\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi)\,(x) :=$$
$$\frac{1}{(2\pi\varepsilon)^{5d/2}} \int_{\mathbb{R}^{5d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} (L^\dagger_{x'})^{k_\xi} \left[e^{\frac{i}{\varepsilon}\Phi^\kappa} (L^\dagger_y)^{k_p} u(x,\xi,x',y,q,p)\varphi(y)\right]\; dq\,dp\,dx'\,d\xi\,dy,$$

where the phase function Φ^κ is given by (4.11) *and the operators $L_y, L_{x'}$ are defined in* (4.12) *and* (1.6)*.*

Again, if the symbol splits as in (5.2), the definition coincides with that of the composition of a PDO and an FIO. We have

5.2 Lemma.

1. *$\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)$ is well-defined.*
2. *If $\sigma \in \mathcal{S}(\mathbb{R}^{3d})$ with $\sigma(0,0) = 1$, we have*
$$[\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi]\,(x) = \lim_{\lambda\to+\infty} \left[\mathcal{R}^\varepsilon\left(\kappa;u^\lambda_\sigma;\Theta^x,\Theta^y\right)\varphi\right](x),$$
where $u^\lambda_\sigma := \sigma(\xi/\lambda, q/\lambda, p/\lambda)u(x,\xi,x',y,q,p)$. The convergence is locally uniform with respect to x.
3. *If $v \in S[+\infty;6d]$ can be written as $v(x,\xi,x',y,q,p) = h(x,\xi)u(x',y,q,p)$ with $u \in S[+\infty;4d]$ and $h \in S[+\infty;2d]$, we have*
$$\mathcal{R}^\varepsilon(\kappa;v;\Theta^x,\Theta^y) = \mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;v;\Theta^x,\Theta^y)$$
as operators on $\mathcal{S}(\mathbb{R}^d)$.
4. *If $u \in S[(+\infty,-\infty,+\infty);(d,d,4d)]$ is independent of ξ, i.e. if there is $v \in S[+\infty;5d]$ such that $u(x,\xi,x',y,q,p) = v(x,x',y,q,p)$, we have*
$$\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y) = \mathcal{I}^\varepsilon(\kappa;w;\Theta^x,\Theta^y)\,.$$
with
$$w(x,y,q,p) = v(x,x,y,q,p).$$

The proofs of the results on the operators $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ are mostly analogue to the corresponding ones on $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$. We will therefore reduce the amount of details provided and refer the reader to Chapter 4 wherever possible.

Proof.

1. Let m be such that $u \in S[(m, m, m, m, m); (d, d, d, d, 2d)]$. By Lemma 10.2, we have
$$\left|\left(L^\dagger_{x'}\right)^k u\right| \leq M^{(x')}_k[\Theta^x, \Theta^y, \varepsilon] \, \langle\xi\rangle^{-k} \sum_{|\alpha|\leq k} |\partial^\alpha_{x'} u| \, .$$
Hence
$$\left|\int_{\mathbb{R}^{5d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} (L^\dagger_{x'})^{k_\xi} \left[e^{\frac{i}{\varepsilon}\Phi^\kappa} (L^\dagger_y)^{k_p} u(x, \xi, x', y, q, p)\varphi(y)\right] \, dq \, dp \, dx' \, d\xi \, dy\right|$$
$$\leq M^{(x')}_k[\Theta^x, \Theta^y, \varepsilon] \left\|\langle\xi\rangle^{-(k_\xi - m_\xi)}\right\|_{L^1(\mathbb{R}^d)}$$
$$\sum_{|\alpha|\leq k_\xi} \sup_{\xi\in\mathbb{R}^d} \left[\left\|\partial^\alpha_{x'} \left[\int_{\mathbb{R}^{4d}} e^{\frac{i}{\varepsilon}\Phi^\kappa} (L^\dagger_y)^{k_p} \frac{u(x, \xi, x', y, q, p)}{\langle\xi\rangle^{m_\xi}} \varphi(y) \, dq \, dp \, dx' \, dy\right]\right\|\right] ,$$
i.e. we have reduced the problem to the estimation of an FIO we encountered in Definition 4.8. Recalling the arguments of the proof of the $\mathcal{S}$-continuity for $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ in Proposition 4.10 we see that the integral in Definition 5.1 is absolutely convergent.

2. The proof of statement 2. is analogue to the corresponding one of Lemma 4.5 and is not shown here.

3. The statement follows directly from the definition.

4. With respect to the last assertion, we notice that we have
$$\left(\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) \, \varphi\right)(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\xi\cdot(x-x')} \left(\mathcal{I}^\varepsilon(\kappa; v; \Theta^x, \Theta^y) \, \varphi\right)(x') \, dx' \, d\xi.$$
Now by Proposition 4.10
$$x' \mapsto \left(\mathcal{I}^\varepsilon(\kappa; v; \Theta^x, \Theta^y) \, \varphi\right)(x')$$
is a Schwartz-class function with respect to x', which is parametrically dependent on x and hence the statement follows by Fourier-inversion.

□

The $\mathcal{S}$-continuity result on $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ translates literally to $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$:

5.3 Proposition. *If $u \in S[+\infty; 6d]$, then $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ is continuous from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^d)$.*

Also the L^2-result extends to the new class of operators

5.4 Theorem. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[0; 6d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$. Then $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$ can be uniquely extended to a bounded operator from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. Moreover there is a constant $C[M^\kappa_0; \Theta^x; \Theta^y]$ sucht that we have the ε-independent bound*

$$\|\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \leq C[M^\kappa_0; \Theta^x; \Theta^y] \max_{\substack{|\alpha|\leq 6d+2 \\ |\beta|\leq 4d+1 \\ |\gamma|\leq 5d+2}} \left\|\partial^\alpha_{(x,y)} \partial^\beta_{x'} \partial^\gamma_\xi u\right\|_{L^\infty(\mathbb{R}^{6d})} . \tag{5.4}$$

The result stated here is not optimal with respect to the order of derivatives one actually needs for the Cotlar-Stein argument. Also the constant $C[M_0^\kappa;\Theta^x;\Theta^y]$ could be made more explicit without adding further insight. The precise statement can be deduced from Proposition 5.9 and shows that the remark concerning the Ehrenfest timescale after Theorem 4.11 also holds for the operators of Theorem 5.4.

We close this section with the analogue of Corollary 4.12. The proof is completely analogous to the one of Corollary 4.12 and thus not repeated.

5.5 Corollary. *Let κ a canonical transformation of class $\mathcal{B}$, $u \in S[0;6d]$, $\Theta^x, \Theta^y \in \mathcal{C}$ and $\alpha, \beta \in \mathbb{N}^d$. We have*

$$\left\| \mathcal{R}^\varepsilon\Big(\kappa; \big(x' - X^\kappa(q,p)\big)^\alpha (y-q)^\beta u; \Theta^x, \Theta^y\Big) \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \tag{5.5}$$

$$\leq C[M_0^\kappa;\Theta^x;\Theta^y]\varepsilon^{\frac{|\alpha|+|\beta|}{2}} \max_{\substack{|\alpha|\leq 6d+2\\|\beta|\leq 4d+1\\|\gamma|\leq 5d+2}} \left\| \partial^\alpha_{(x,y)}\partial^\beta_{x'}\partial^\gamma_\xi u\right\|_{L^\infty(\mathbb{R}^{6d})} \tag{5.6}$$

5.2 Proofs

We present the proofs of Proposition 5.3 and Theorem 5.4. Whereas the generalisation of the $\mathcal{S}$-continuity only adds some technicalities, additional twists will be needed to prove the L^2-boundedness.

5.2.1 Reduction to a generic case

Again, we have a rescaling, which allows for a simplification of the proofs. We have

5.6 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[m;6d]$ and $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$ real symmetric. Setting*

$$u^{(\varepsilon)}(x,\xi,x',y,q,p) := u(\sqrt{\varepsilon}x, \sqrt{\varepsilon}\xi, \sqrt{\varepsilon}x', \sqrt{\varepsilon}y, \sqrt{\varepsilon}q, \sqrt{\varepsilon}p),$$

we have

1. *$u^{(\varepsilon)} \in S^{-1/2}[m;6d]$ and*
$$\left\|\partial^\alpha_{(x,y)}\partial^\beta_{(x',\xi)}u^{(\varepsilon)}\right\|_{L^\infty(\mathbb{R}^{6d})} = \varepsilon^{|\alpha+\beta|/2}\left\|\partial^\alpha_{(x,y)}\partial^\beta_{(x',\xi)}u\right\|_{L^\infty(\mathbb{R}^{6d})} \tag{5.7}$$
if $u \in S[0;6d]$.
2. *$\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y) = (D[\varepsilon])^* \circ \mathcal{R}^1\big(\kappa^{(\varepsilon)};u^{(\varepsilon)};\Theta^x,\Theta^y\big)\circ D[\varepsilon]$.*

for the rescaling in ε and

5.7 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$, $u \in S[m;6d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$ with lower bounds Θ^x_0 and Θ^y_0. Defining*

$$v^\varepsilon = w\left(\varepsilon^{-\frac12}(x'-X^\kappa(q,p)), \varepsilon^{-\frac12}(y-q), q, p\right)u,$$

with

$$w(x',y,q,p) = \exp\left[-\left[(\Theta^x(q,p)-\Theta^x_0)^{\frac12}\,x'\right]^2/2\right]\exp\left[-\left[(\Theta^y(q,p)-\Theta^y_0)^{\frac12}\,y\right]^2/2\right]$$

we have

1. $v^\varepsilon \in S^{1/2}[m; 6d]$ *and*

$$\left\| \partial^\alpha_{(x,y)} \partial^\beta_{(x',\xi)} u^{(\varepsilon)} \right\|_{L^\infty(\mathbb{R}^{6d})} \leq C[\Theta^x, \Theta^y] \left\| \partial^\alpha_{(x,y)} \partial^\beta_{(x',\xi)} u \right\|_{L^\infty(\mathbb{R}^{6d})}$$

for $u \in S[0; 6d]$.

2. $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) = \mathcal{R}^\varepsilon(\kappa; v^\varepsilon; \Theta^x_0, \Theta^y_0)$.

for the reduction to $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$. The proofs of these lemmas are completely analogous to the ones of Lemmas 4.14 and 5.7.

5.2.2 Proof of the continuity on $\mathcal{S}(\mathbb{R}^d)$

In a first step, we provide a technical lemma, which allows for the conversion of growth in x and ξ to growth in x', q and p.

5.8 Lemma. *Let* $u \in S[+\infty; 6d]$ *and* $\varphi \in \mathcal{S}(\mathbb{R}^d)$. *We have*

$$\left[\mathcal{R}^1\big(\kappa; V \cdot (x - x')u; \Theta^x_0, \Theta^y_0\big)\,\varphi\right](x) = i\left[\mathcal{R}^1(\kappa; V \cdot \nabla_\xi u; \Theta^x_0, \Theta^y_0)\,\varphi\right](x) \tag{5.8}$$

and

$$\begin{aligned} &\left[\mathcal{R}^1(\kappa; V \cdot (\xi - \Xi^\kappa(q,p))u; \Theta^x_0, \Theta^y_0)\,\varphi\right](x) \\ &= i\left[\mathcal{R}^1\big(\kappa; V \cdot \left[\Theta^x_0(x' - X^\kappa(q,p))\right] u; \Theta^x_0, \Theta^y_0\big)\,\varphi\right](x) - i\left[\mathcal{R}^1(\kappa; V \cdot \nabla_{x'} u; \Theta^x_0, \Theta^y_0)\,\varphi\right](x) \end{aligned} \tag{5.9}$$

Proof. We have

$$\begin{pmatrix} \nabla_\xi \Psi^\kappa \\ \nabla_{x'} \Psi^\kappa \end{pmatrix} = \begin{pmatrix} x - x' \\ \Xi^\kappa(q,p) - \xi + i\Theta^x_0(x' - X^\kappa(q,p)) \end{pmatrix}.$$

Thus the result follows by integration by parts:

$$\begin{aligned} &(2\pi\varepsilon)^{5d/2}\mathcal{R}^1\big(\kappa; V \cdot (x - x')u; \Theta^x_0, \Theta^y_0\big)\,\varphi(x) \\ &= \lim_{\lambda\to\infty} \int_{\mathbb{R}^{5d}} e^{i\Psi^\kappa}\sigma(\xi/\lambda, p/\lambda)\,\big(V \cdot (x - x')u\varphi(y)\big)\; dq\,dp\,dx'\,d\xi\,dy \\ &= \lim_{\lambda\to\infty} \int_{\mathbb{R}^{5d}} e^{i\Psi^\kappa}\sigma(\xi/\lambda, p/\lambda)\,(iV \cdot \nabla_\xi u\varphi(y))\; dq\,dp\,dx'\,d\xi\,dy \\ &\quad + \lim_{\lambda\to\infty} \int_{\mathbb{R}^{5d}} e^{i\Psi^\kappa}\lambda^{-1}\,(iV \cdot \nabla_\xi\sigma(\xi/\lambda, p/\lambda))\,(u\varphi(y))\; dq\,dp\,dx'\,d\xi\,dy \\ &= \big(\mathcal{R}^1(\kappa; iV \cdot \nabla_\xi u; \Theta^x, \Theta^y)\,\varphi\big)(y), \end{aligned}$$

where the last equality holds by dominated convergence, as

$$\lim_{\lambda\to\infty}\big(\lambda^{-1}\nabla_\xi\sigma(\xi/\lambda, p/\lambda)\big) = 0 \qquad \forall p, \xi \in \mathbb{R}^d.$$

The proof of the second equality follows analogously. □

Proof of Proposition 5.3.

Let m be such that $u \in S[(2m, 2m, 2m, 2m, 2m); (d, d, d, d, 2d)]$. We have

$$\begin{aligned}
&(2\pi)^{5d/2}\partial_x^\beta \left[\mathcal{R}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\,\varphi\right](x)\\
&= \lim_{\lambda\to\infty} \partial_x^\beta \int_{\mathbb{R}^{5d}} e^{i\Psi^\kappa} u_\sigma^\lambda(x, \xi, x', y, q, p)\varphi(y)\; dq\, dp\, dx'\, d\xi\, dy\\
&= \sum_{\gamma\le\beta} \binom{\beta}{\gamma} \lim_{\lambda\to\infty} \int_{\mathbb{R}^{5d}} \xi^{\beta-\gamma} e^{i\Psi^\kappa} \partial_x^\gamma u_\sigma^\lambda(x, \xi, x', y, q, p)\varphi(y)\; dq\, dp\, dx'\, d\xi\, dy.
\end{aligned}$$

Thus the required smoothness of the expression by the local uniformity of the convergence. Using (5.8), we see that

$$\begin{aligned}
&\int_{\mathbb{R}^{5d}} \langle x\rangle^{2m} x^\alpha \xi^{\beta-\gamma} e^{i\Psi^\kappa} \frac{\partial_x^\gamma u_\sigma^\lambda(x, \xi, x', y, q, p)}{\langle x\rangle^{2m}} \varphi(y) \;\; dq\, dp\, dx'\, d\xi\, dy\\
&= \sum_{|\delta|\le|\alpha|+2m} \int_{\mathbb{R}^{5d}} P^{\alpha\beta\gamma\delta}(x', \xi) e^{i\Psi^\kappa} \frac{\partial_x^\gamma \partial_\xi^\delta u_\sigma^\lambda(x, \xi, x', y, q, p)}{\langle x\rangle^{2m}\langle \xi\rangle^{2m}} \varphi(y) \;\; dq\, dp\, dx'\, d\xi\, dy
\end{aligned}$$

where $P^{\alpha\beta\gamma}$ is polynomial in x' (of degree $|\alpha| + 2m$) and ξ (of degree $|\beta - \gamma| + 2m$). For better readability, we will drop the arguments of $X^\kappa(q, p)$ and $\Xi^\kappa(q, p)$ in what follows.

Reexpanding $P^{\alpha\beta\gamma}$ in $(\xi - \Xi^\kappa)$ and using (5.9), we see that the terms in the last sum may be estimated by

$$\begin{aligned}
&\sum_{\rho\le|\beta-\gamma|+2m+2d+2} \int_{\mathbb{R}^{2d}} \frac{1}{\langle x'\rangle^{2d+2}\langle \xi\rangle^{2d+2}}\; dx'\, d\xi\\
&\sup_{x,x',\xi\in\mathbb{R}^d} \left| \int_{\mathbb{R}^{3d}} Q^{\alpha\beta\gamma\delta\rho}(x', \Xi^\kappa, x' - X^\kappa) e^{i\Phi^\kappa} \frac{\partial_{x'}^\rho \partial_x^\gamma \partial_\xi^\delta u(x, \xi, x', y, q, p)}{\langle x\rangle^{2m}\langle \xi\rangle^{2m}} \varphi(y)\; dq\, dp\, dy \right|
\end{aligned}$$

where $Q^{\alpha\beta\gamma\delta\rho}$ is polynomial of degree $|\alpha| + 2m + 2d + 2$ with respect to x' and of degree $|\beta - \gamma| + 2m + 2d + 2$ with respect to Ξ^κ and $x' - X^\kappa$.

Now the x'-supremum in the last expression is the $\|\cdot\|_{00}$ semi-norm of

$$\mathcal{I}^\varepsilon\left(\kappa; v_{x,\xi}^\varepsilon; \Theta_0^x, \Theta_0^y\right)\varphi,$$

where the symbol

$$v_{x,\xi}^\varepsilon(x', y, q, p) = Q^{\alpha\beta\gamma\delta\rho}(x', \Xi^\kappa, x' - X^\kappa) \frac{\partial_{x'}^\rho \partial_x^\gamma \partial_\xi^\delta u(x, \xi, x', y, q, p)}{\langle x\rangle^{2m}\langle \xi\rangle^{2m}} \tag{5.10}$$

depends parametrically on x and ξ and is in the class $S[(2m_{\alpha\beta m}, 2m_{\alpha\beta m}, 2m_{\alpha\beta m}); (d, d, 2d)]$, where $m_{\alpha\beta m} = |\alpha| + 2\,|\beta| + 6m + 6d + 6$.

In Equation (4.24) of the proof of Proposition 4.10, we established the bound

$$\begin{aligned}
&\left\|\mathcal{I}^\varepsilon(\kappa; v_{x,\xi}; \Theta_0^x, \Theta_0^y)\,\varphi\right\|_{00}\\
&\le C_{\alpha\beta}[\Theta_0^x, \Theta_0^y] \sum_{|\alpha'|\le 4m_{\alpha\beta m}+2d+2} \left\| \frac{\partial_{(x',y)}^{\alpha'} v_{x,\xi}}{(\langle x'\rangle\,\langle y\rangle\,\langle (q,p)\rangle)^{2m_{\alpha\beta m}}} \right\|_{L^\infty(\mathbb{R}^{4d})} \sum_{\substack{|\alpha'|\le 6m_{\alpha\beta m}+3d+3\\ |\beta'|\le 4m_{\alpha\beta m}+2d+2}} \|\varphi\|_{\alpha'\beta'}\,.
\end{aligned}$$

Now, taking the explicit form of $v^{\varepsilon}_{x,\xi}$ in (5.10) into account and noting that

$$\left\| \frac{\partial^{\alpha'}_{x'} \left[Q^{\alpha\beta\gamma\delta\rho}(x', \Xi^{\kappa}, x' - X^{\kappa}) \right]}{(\langle x' \rangle \langle (q,p) \rangle)^{|\alpha|+2|\beta|+4m+6d+6}} \right\|_{L^{\infty}(\mathbb{R}^{3d})} < \infty,$$

we have established the bound

$$\left\| \mathcal{R}^1(\kappa; u; \Theta^x_0, \Theta^y_0)\, \varphi \right\|_{\alpha\beta} \leq C_{\alpha\beta}[\Theta^x_0, \Theta^y_0] \sum_{\gamma'} \left\| \frac{\partial^{\gamma'}_{(x,\xi,x',y)} u}{(\langle x' \rangle \langle y \rangle \langle (q,p) \rangle)^{2m}} \right\|_{L^{\infty}(\mathbb{R}^{4d})} \sum_{\alpha'\beta'} \|\varphi\|_{\alpha'\beta'},$$

where the sums are taken over

$$\begin{aligned} \left|\gamma'\right| &\leq 4m_{\alpha\beta m} + |\alpha| + 2\,|\beta| + 4m + 4d + 4 \\ \left|\alpha'\right| &\leq 6m_{\alpha\beta m} + 3d + 3 \\ \left|\beta'\right| &\leq 4m_{\alpha\beta m} + 2d + 2. \end{aligned}$$

□

5.2.3 Proof of the continuity on $L^2(\mathbb{R}^d)$

We start with the proof of the L^2-bound, which follows the same strategy as the proof of Theorem 4.11, i.e. we will first prove a result on FIOs with compactly supported symbols with help of the Schur Lemma. In a second step, the L^2-bound for general symbols will follow from the Cotlar-Stein Lemma.

Estimate on FIOs with compactly supported symbols

5.9 Proposition. *Let κ be a canonical transformation of class $\mathcal{B}$, $\Theta^x_0, \Theta^y_0 \in \mathcal{C}_{\mathrm{const}}$ and and $u, v \in S[(0,-\infty,0,-\infty);(d,d,2d,2d)]$ be compactly supported in ξ and (q,p) independently of x, x' and y, i.e.* $\operatorname{supp} u \subset \mathbb{R}^d \times K'_u \times \mathbb{R}^{2d} \times K_u$ *and* $\operatorname{supp} v \subset \mathbb{R}^d \times K'_u \times \mathbb{R}^{2d} \times K_u$*, where K'_u and K'_v are compact subsets of $\mathbb{R}^d$ and K_u and K_v are compact subsets of $\mathbb{R}^{2d}$. Then, for any $l_1, l_2 \in \mathbb{N}$,*

$$\begin{aligned} &\left\| \mathcal{R}^1(\kappa; v; \Theta^x_0, \Theta^y_0)\, \mathcal{R}^1(\kappa; u; \Theta^x_0, \Theta^y_0)^* \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \qquad (5.11)\\ &\leq \frac{C_{l_1,l_2}}{\det \Theta^x_0\, (\det \Theta^y_0)^{1/2}} \left\langle \delta_{\Lambda[\Theta^y_0]}(K_u, K_v) \right\rangle^{-l_1} \left\langle \delta(K'_u, K'_v)/2 \right\rangle^{-l_2} \min\left[(\lambda^x)^{-\frac{1}{2}}, c_{\Lambda[\Theta^y_0]\circ\kappa^{-1}} \right]^{-\min(l_1,l_2)/2} \\ &\quad \min(1, \lambda^x, \lambda^y)^{-\frac{l_1+2l_2}{2}} \sum_{\substack{\alpha_1+\beta_1\leq l_1+l_2 \\ \alpha_2+\beta_2\leq l_2 \\ \alpha_3+\beta_3\leq d+1}} \left\| \partial^{\alpha_1}_y \partial^{\alpha_2}_{x'} \partial^{\alpha_3}_{\xi} u \right\|_{L^{\infty}_{(x,x',y)} L^1_{(\xi,q,p)}} \left\| \partial^{\beta_1}_y \partial^{\beta_2}_{x'} \partial^{\beta_3}_{\xi} v \right\|_{L^{\infty}_{(x,x',y)} L^1_{(\xi,q,p)}} \end{aligned}$$

and

$$\begin{aligned} &\left\| \mathcal{R}^1(\kappa; v; \Theta^x_0, \Theta^y_0)^*\, \mathcal{R}^1(\kappa; u; \Theta^x_0, \Theta^y_0) \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \qquad (5.12)\\ &\leq \frac{C_{l_1,l_2}}{\det \Theta^x_0\, (\det \Theta^y_0)^{1/2}} \left\langle \delta_{\Lambda[\Theta^x_0]\circ\kappa}(K_u, K_v) \right\rangle^{-l_1} \left\langle \delta(K'_u, K'_v) \right\rangle^{-l_2} \min(1, \Lambda[\Theta^x_0])^{\frac{l_1+d+1}{2}} \\ &\quad \sum_{\substack{\alpha_1+\beta_1\leq l_2 \\ \alpha_2+\beta_2\leq l_1 \\ \alpha_3+\beta_3\leq l_1 \\ \alpha_4+\beta_4\leq d+1}} \left\| \partial^{\alpha_1+\alpha_3}_x \partial^{\alpha_2+\alpha_4}_{\xi} \partial^{\alpha_3}_{x'} u \right\|_{L^{\infty}_{(x,x',y)} L^1_{(\xi,q,p)}} \left\| \partial^{\beta_1+\beta_3}_x \partial^{\beta_2+\beta_4}_{\xi} \partial^{\beta_3}_{x'} v \right\|_{L^{\infty}_{(x,x',y)} L^1_{(\xi,q,p)}}. \end{aligned}$$

Proof. The proof follows the same strategy as the one of Theorem 4.11. However because of the asymmetric structure of the phase function, we will have to estimate $\mathcal{R}\mathcal{R}^*$ and $\mathcal{R}^*\mathcal{R}$ separately.

Estimate on $\mathcal{R}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\, \mathcal{R}^1(\kappa; v; \Theta_0^x, \Theta_0^y)^*$

We have

$$(2\pi)^{5d}\mathcal{R}^1(\kappa; u; \Theta_0^x, \Theta_0^y)\, \mathcal{R}^1(\kappa; v; \Theta_0^x, \Theta_0^y)^*\, \varphi(x) = \int_{\mathbb{R}^d} K(x,y)\varphi(y)\, dy,$$

where the integral kernel $K(x,y)$ is given by the absolutely convergent integral

$$\int_{\mathbb{R}^{9d}} e^{i\Omega^\kappa} u(x, \xi_1, x_1', w, q_1, p_1)\overline{v(y, \xi_2, x_2', w, q_2, p_2)}\, dq_1\, dq_2\, dp_1\, dp_2\, dx_1'\, dx_2'\, d\xi_1\, d\xi_2\, dw$$

with phase function

$$\begin{aligned}
&\Omega^\kappa(x, y, w, x_1', x_2', \xi_1, \xi_2, q_1, q_2, p_1, p_2; \Theta_0^x, \Theta_0^y)\\
&= \Psi^\kappa(x, \xi_1, x_1', w, q_1, p_1; \Theta_0^x, \Theta_0^y) - \overline{\Psi^\kappa(y, \xi_2, x_2', w, q_2, p_2; \Theta_0^x, \Theta_0^y)}.
\end{aligned}$$

Using the linear transformations defined by

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \begin{pmatrix} \hat{x} + \delta_x/2 \\ \hat{x} - \delta_x/2 \end{pmatrix}, \qquad \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \begin{pmatrix} \hat{\xi} + \delta_\xi/2 \\ \hat{\xi} - \delta_\xi/2 \end{pmatrix},$$

we have

$$\begin{aligned}
&\Omega^\kappa(x, y, w, x_1', x_2', \xi_1, \xi_2, q_1, q_2, p_1, p_2; \Theta_0^x, \Theta_0^y)\\
&= (x - (\hat{x} + \delta_x/2)) \cdot (\hat{\xi} + \delta_\xi/2) - (y - (\hat{x} - \delta_x/2)) \cdot (\hat{\xi} - \delta_\xi/2)\\
&\quad + S^\kappa(q_1, p_1) - S^\kappa(q_2, p_2) - p_1 \cdot (w - q_1) + p_2 \cdot (w - q_2)\\
&\quad + \Xi^\kappa(q_1, p_1) \cdot (\hat{x} + \delta_x/2 - X^\kappa(q_1, p_1)) - \Xi^\kappa(q_2, p_2) \cdot (\hat{x} - \delta_x/2 - X^\kappa(q_2, p_2))\\
&\quad + i\Theta_0^x \left((\hat{x} + \delta_x/2) - X^\kappa(q_1, p_1)\right)^2/2 + i\Theta_0^x \left((\hat{x} - \delta_x/2) - X^\kappa(q_2, p_2)\right)^2/2\\
&\quad + i\Theta_0^y\, (w - q_1)^2/2 + i\Theta_0^y\, (w - q_2)^2/2.
\end{aligned}$$

Thus

$$\begin{aligned}
\Im\Omega^\kappa &= \Theta_0^y \left(w - \frac{q_1 + q_2}{2}\right)^2 + \Theta_0^y \left(\frac{q_1 - q_2}{2}\right)^2\\
&\quad + \Theta_0^x \left(\hat{x} - \frac{X^\kappa(q_1, p_1) + X^\kappa(q_2, p_2)}{2}\right)^2 + \Theta_0^x \left([X^\kappa]_{(q_2,p_2)}^{(q_1,p_1)} - \delta_x\right)^2/4
\end{aligned}$$

and

$$\nabla_{(w,\hat{x},\hat{\xi})}\Omega^\kappa = \begin{pmatrix} p_2 - p_1 + 2i\Theta_0^y \left(w - \frac{q_1+q_2}{2}\right) \\ -\delta_\xi + [\Xi^\kappa]_{(q_2,p_2)}^{(q_1,p_1)} + 2i\Theta_0^x \left(\hat{x} - \frac{X^\kappa(q_1,p_1)+X^\kappa(q_2,p_2)}{2}\right) \\ x - y - \delta_x \end{pmatrix},$$

where we used the notation

$$[X^\kappa]_{(q_2,p_2)}^{(q_1,p_1)} := X^\kappa(q_1, p_1) - X^\kappa(q_2, p_2), \qquad [\Xi^\kappa]_{(q_2,p_2)}^{(q_1,p_1)} := \Xi^\kappa(q_1, p_1) - \Xi^\kappa(q_2, p_2).$$

We introduce the first order differential operators

$$L_w = \frac{1 - i\,(\Theta_0^y)^{-1}\,\overline{\nabla_w \Omega^\kappa}\cdot\nabla_w}{1+\left|(\Theta_0^y)^{-1/2}\,\nabla_w\Omega^\kappa\right|^2}, \quad L_{\hat{x}} = \frac{1 - i\,(\Theta_0^x)^{-1}\,\overline{\nabla_{\hat{x}} \Omega^\kappa}\cdot\nabla_{\hat{x}}}{1+\left|(\Theta_0^x)^{-1/2}\,\nabla_{\hat{x}}\Omega^\kappa\right|^2}$$

and

$$L_{\hat{\xi}} = \frac{1 - i\overline{\nabla_{\hat{\xi}}\Omega^\kappa}\cdot\nabla_{\hat{\xi}}}{1+\left|\nabla_{\hat{\xi}}\Omega^\kappa\right|^2}.$$

They commute and fulfill

$$L_* e^{i\Omega^\kappa} = e^{i\Omega^\kappa},$$

where $*$ stands for $\hat{\xi}, w$ or $\hat{x}$. Moreover, they provide decay

$$\left|\left(L_w^\dagger\right)^{l_1}(u\overline{v})\right| \le \frac{M_{l_1}^{(w)}}{\left\langle(\Theta_0^y)^{-1/2}\,(p_2-p_1)\right\rangle^{l_1}} \sum_{|\alpha|\le l_1}\left|\left[(\Theta_0^y)^{-1/2}\,\nabla_w\right]^\alpha(u\overline{v})\right|$$

$$\left|\left(L_{\hat{x}}^\dagger\right)^{l_2}(u\overline{v})\right| \le \frac{M_{l_2}^{(\hat{x})}}{\left\langle(\Theta_0^x)^{-1/2}\left[\delta_\xi - [\Xi^\kappa]_{(q_2,p_2)}^{(q_1,p_1)}\right]\right\rangle^{l_2}} \sum_{|\alpha|\le l_2}\left|\left[(\Theta_0^x)^{-1/2}\,\nabla_{\hat{x}}\right]^\alpha(u\overline{v})\right|$$

$$\left|\left(L_{\hat{\xi}}^\dagger\right)^{l_3}(u\overline{v})\right| = \left|\left(\frac{1+i(x-y-\delta_x)\cdot\nabla_{\hat{\xi}}}{1+|x-y-\delta_x|^2}\right)^{l_3}(u\overline{v})\right| \le \frac{M_{l_3}^{(\hat{\xi})}}{\langle x-y-\delta_x\rangle^{l_3}}\sum_{|\alpha|\le l_3}\left|\partial_{\hat{\xi}}^\alpha(u\overline{v})\right|,$$

compare Lemma 10.2 in the appendix.

Hence we have

$$\begin{aligned}
&|K(x,y)| \\
&= \left|\int_{\mathbb{R}^{9d}} e^{i\Omega^\kappa}\left(L_w^\dagger\right)^{(l_1+l_1')}\left(L_{\hat{x}}^\dagger\right)^{l_2}\left(L_{\hat{\xi}}^\dagger\right)^{l_3}(u\overline{v})\ dq_1'\,dq_2'\,dp_1'\,dp_2'\,d\hat{x}\,d\delta_x\,d\hat{\xi}\,d\delta_\xi\,dw\right| \\
&\le M_{l_1+l_1'}^{(w)} M_{l_2}^{(\hat{x})} M_{l_3}^{(\hat{\xi})} \qquad (5.13)\\
&\int_{\mathbb{R}^{9d}}\left\langle(\Theta_0^y)^{-\frac{1}{2}}\,(p_2-p_1)\right\rangle^{-(l_1+l_1')}\left\langle(\Theta_0^x)^{-\frac{1}{2}}\left[\delta_\xi-[\Xi^\kappa]_{(q_2,p_2)}^{(q_1,p_1)}\right]\right\rangle^{-l_2} \\
&\quad\times\langle x-y-\delta_x\rangle^{-l_3}\, e^{-\Theta_0^y\left(w-\frac{q_1+q_2}{2}\right)^2} e^{-\Theta_0^x\left[\hat{x}-\frac{1}{2}[X^\kappa(q_1,p_1)+X^\kappa(q_2,p_2)]\right]^2} \\
&\quad\times e^{-\Theta_0^x\left(\delta_x-[X^\kappa]_{(q_2,p_2)}^{(q_1,p_1)}\right)^2/4} e^{-\Theta_0^y\left(\frac{q_1-q_2}{2}\right)^2} \\
&\quad\times\sum_{\substack{\alpha\le(l_1+l_1')\\ \beta\le l_2\\ \gamma\le l_3}}\left|\left[(\Theta_0^y)^{-\frac{1}{2}}\,\nabla_w\right]^\alpha\left[(\Theta_0^x)^{-\frac{1}{2}}\,\nabla_{\hat{x}}\right]^\beta\partial_{\hat{\xi}}^\gamma\,(u\overline{v})\right|\ dq_1'\,dq_2'\,dp_1'\,dp_2'\,d\hat{x}\,d\delta_x\,d\hat{\xi}\,d\delta_\xi\,dw
\end{aligned}$$

To get convergence of the y-integral in the integral over the kernel, we choose $l_3 = d+1$. After the y integral, we perform the $w, \hat{x}$ and δ_x integrals and are left with

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d} |K(x,y)|\ dy \\
&\leq C \left\| \langle y\rangle^{-l_3} \right\|_{L^1(\mathbb{R}^d)} \left\| e^{-\Theta_0^y w^2} \right\|_{L^1(\mathbb{R}^d)} \left\| e^{-\Theta_0^x \hat{x}^2} \right\|_{L^1(\mathbb{R}^d)} \left\| e^{-\Theta_0^x \delta_x^2/4} \right\|_{L^1(\mathbb{R}^d)} \left\| e^{-q^2/4} \langle q\rangle^{l_1+l_1'} \right\|_{L^\infty(\mathbb{R}^d)} \\
&\int_{\mathbb{R}^{9d}} \left\langle \Lambda[\Theta_0^y] \left((q_1,p_1)-(q_2,p_2)\right)^\dagger \right\rangle^{-(l_1+l_1')} \left\langle (\Theta_0^x)^{-\frac{1}{2}} \left[\delta_\xi - [\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right] \right\rangle^{-l_2} \\
&\quad \sum_{\substack{\alpha\leq(l_1+l_1')\\ \beta\leq l_2\\ \gamma\leq d+1}} \left\| \left[(\Theta_0^y)^{-\frac{1}{2}}\nabla_w\right]^\alpha \left[(\Theta_0^x)^{-\frac{1}{2}}\nabla_{\hat{x}}\right]^\beta \partial_{\hat{\xi}}^\gamma (u\overline{v}) \right\|_{L^\infty_{(x,y,w,\hat{x},\delta_x)}} dq_1'\, dq_2'\, dp_1'\, dp_2'\, d\hat{\xi}\, d\delta_\xi,
\end{aligned}$$

where we wrote

$$e^{-\Theta_0^y\left(\frac{q_1-q_2}{2}\right)^2} = e^{-\Theta_0^y\left(\frac{q_1-q_2}{2}\right)^2} \left\langle (\Theta_0^y)^{\frac{1}{2}}(q_1-q_2)/2 \right\rangle^{l_1+l_1'} \left\langle (\Theta_0^y)^{\frac{1}{2}}(q_1-q_2)/2 \right\rangle^{-(l_1+l_1')}$$

to get the decay in $(\Theta_0^y)^{\frac{1}{2}}(q_1-q_2)/2$. Moreover, because of the symmetry of (5.13), we have exactly the same estimate for $\sup_{y\in\mathbb{R}^d}\int |K(x,y)|\ dx$.

To get the decay in $\delta(K_u', K_v')$, we split the ξ-integral into the two regions

1. $K_> := \{\delta_\xi : |\delta_\xi| > 2\,|\Xi^\kappa(q_1,p_1) - \Xi^\kappa(q_2,p_2)|\} \subset \mathbb{R}^d$ and

2. $K_\leq := \{\delta_\xi : |\delta_\xi| \leq 2\,|\Xi^\kappa(q_1,p_1) - \Xi^\kappa(q_2,p_2)|\} \subset \mathbb{R}^d$,

where we suppressed the dependence of the sets on the phase-space variables in the notation.

In $K_>$ we have

$$\left|\delta_\xi - [\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right| \geq \left| |\delta_\xi| - \left|[\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right| \right| \geq |\delta_\xi|/2,$$

and thus

$$\left\langle (\Theta_0^x)^{-\frac{1}{2}} \left[\delta_\xi - [\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right] \right\rangle^{-l_2} \leq \left\langle (\lambda^x)^{-\frac{1}{2}}\delta_\xi/2 \right\rangle^{-l_2}$$

whereas the elements of $K_\leq$ fulfill

$$c_{\Lambda[\Theta_0^y]\circ\kappa^{-1}} |\delta_\xi| \leq 2c_{\Lambda[\Theta_0^y]\circ\kappa^{-1}} |\kappa(q_1,p_1) - \kappa(q_2,p_2)| \leq 2\left\|\Lambda[\Theta_0^y]\left((q_1,p_1)-(q_2,p_2)\right)\right\|,$$

which gives the estimate

$$\langle \Lambda[\Theta_0^y]\left((q_1,p_1)-(q_2,p_2)\right)\rangle^{-l_1'} \leq \left\langle c_{\Lambda[\Theta_0^y]\circ\kappa^{-1}}\delta_\xi/2 \right\rangle^{-l_1'}.$$

Adding the trivial estimate $\langle x\rangle^{-1} \le 1$, we continue with

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y)|\ dy \\
&\le C' \left(\det \Theta_0^x\right)^{-1} \left(\det \Theta_0^y\right)^{-\frac{1}{2}} \sum_{\substack{\alpha\le(l_1+l_1')\\ \beta\le l_2\\ \gamma\le d+1}} (\lambda^x)^{-\frac{|\alpha|}{2}} (\lambda^y)^{-\frac{|\beta|}{2}} \int \left\langle \Lambda[\Theta_0^y]\left((q_1,p_1)-(q_2,p_2)\right)^\dagger \right\rangle^{-l_1} \\
&\left[\int_{K_>} \left\langle (\lambda^x)^{-\frac{1}{2}} \delta_\xi/2 \right\rangle^{-l_2} \left\| \partial_w^\alpha \partial_{\hat{x}}^\beta \partial_{\hat{\xi}}^\gamma \left(u\overline{v}\right)\right\|_{L^\infty_{(x,y,w,\hat{x},\delta_x)}} d\delta_\xi \right.\\
&\quad \left. + \int_{K_\le} \left\langle c_{\Lambda[\Theta_0^y]\circ\kappa^{-1}} \delta_\xi/2 \right\rangle^{-l_1'} \left\| \partial_w^\alpha \partial_{\hat{x}}^\beta \partial_{\hat{\xi}}^\gamma \left(u\overline{v}\right)\right\|_{L^\infty_{(x,y,w,\hat{x},\delta_x)}} d\delta_\xi \right] dq_1\, dp_1\, dq_2\, dp_2\, d\hat{\xi} \\
&\le C'' \frac{(\det\Theta_0^x)^{-1}(\det\Theta_0^y)^{-\frac{1}{2}} \left\langle \delta_{\Lambda[\Theta_0^y]}\left(K_u,K_v\right)\right\rangle^{-l_1}}{\left\langle \min\left[(\lambda^x)^{-\frac{1}{2}}, c_{\Lambda[\Theta_0^y]\circ\kappa^{-1}}\right] \delta(K_u',K_v')/2 \right\rangle^{\min(l_2,l_1')}} \\
&\quad \sum_{\substack{\alpha\le(l_1+l_1')\\ \beta\le l_2\\ \gamma\le d+1}} (\lambda^x)^{-\frac{|\alpha|}{2}} (\lambda^y)^{-\frac{|\beta|}{2}} \int \left\| \partial_w^\alpha \partial_{\hat{x}}^\beta \partial_{\hat{\xi}}^\gamma \left(u\overline{v}\right)\right\|_{L^\infty_{(x,y,w,\hat{x},\delta_x)}} d\delta_\xi\, dq_1\, dp_1\, dq_2\, dp_2\, d\hat{\xi}
\end{aligned}$$

Recalling the arguments of u and v, we have

$$\begin{aligned}
&\int_{\mathbb{R}^{6d}} \left| \partial_w^\alpha \partial_{\hat{x}}^\beta \partial_{\hat{\xi}}^\gamma \left[u^\kappa(x,\hat{\xi}+\delta_\xi,\hat{x}+\delta_x,w,q_1',p_1') \right.\right.\\
&\qquad\qquad \left.\left. \overline{v^\kappa(y,\hat{\xi}-\delta_\xi,\hat{x}-\delta_x,w,q_2',p_2')}\right]\right| dq_1\, dq_2\, dp_1\, dp_2\, d\hat{\xi}\, d\delta_\xi \\
&= \sum_{\substack{\alpha_1+\alpha_2=\alpha\\ \beta_1+\beta_2=\beta\\ \gamma_1+\gamma_2=\gamma}} \binom{\alpha}{\alpha_1}\binom{\beta}{\beta_2}\binom{\gamma}{\gamma_1} \int_{\mathbb{R}^{3d}} \left| \partial_w^{\alpha_1} \partial_{x_1'}^{\beta_1} \partial_{\xi_1}^{\gamma_1} u(x,\xi_1,x_1',w,q_1',p_1')\right| dq_1\, dp_1\, d\xi_1 \\
&\qquad \int_{\mathbb{R}^{3d}} \left| \partial_w^{\alpha_2} \partial_{x_2'}^{\beta_2} \partial_{\xi_2}^{\gamma_2} v(x,\xi_2,x_2',w,q_2',p_2')\right| dq_2\, dp_2\, d\xi_2 \\
&\le 2^{|\alpha|+|\beta|+|\gamma|} \left\| \partial_y^{\alpha_1} \partial_{x'}^{\beta_1} \partial_\xi^{\gamma_1} u \right\|_{L^\infty_{(x,x',y)} L^1(\xi,q,p)} \left\| \partial_y^{\alpha_2} \partial_{x'}^{\beta_2} \partial_\xi^{\gamma_2} v \right\|_{L^\infty_{(x,x',y)} L^1(\xi,q,p)}
\end{aligned}$$

and thus the first part of the result.

Estimate on $\mathcal{R}^1(\kappa;u;\Theta_0^x,\Theta_0^y)^*\, \mathcal{R}^1(\kappa;v;\Theta_0^x,\Theta_0^y)$

We have

$$(2\pi)^{5d} \mathcal{R}^1(\kappa;u;\Theta_0^x,\Theta_0^y)^*\, \mathcal{R}^1(\kappa;v;\Theta_0^x,\Theta_0^y)\, \varphi(x) = \int_{\mathbb{R}^d} K(x,y)\varphi(y)\ dy,$$

where the integral kernel $K(x,y)$ is given by the oscillatory integral

$$\int_{\mathbb{R}^{9d}} e^{i\Omega^\kappa} \overline{u(w,\xi_1,x_1',x,q_1,p_1)} v(w,\xi_2,x_2',y,q_2,p_2)\ dq_1\, dq_2\, dp_1\, dp_2\, dx_1'\, dx_2'\, d\xi_1\, d\xi_2\, dw$$

with the phase function

$$
\begin{aligned}
&\Omega^\kappa(x, y, w, x_1', x_2', \xi_1, \xi_2, q_1, q_2, p_1, p_2; \Theta_0^x, \Theta_0^y) \\
&= -\overline{\Psi^\kappa(w, \xi_1, x_1', x, q_1, p_1; \Theta_0^x, \Theta_0^y)} + \Psi^\kappa(w, \xi_2, x_2', y, q_2, p_2; \Theta_0^x, \Theta_0^y) \\
&= (w - (\hat{x} - \delta_x/2)) \cdot (\hat{\xi} - \delta_\xi/2) - (w - (\hat{x} + \delta_x/2)) \cdot (\hat{\xi} + \delta_\xi/2) \\
&\quad + S^\kappa(q_2, p_2) - S^\kappa(q_1, p_1) - p_2 \cdot (y - q_2) + p_1 \cdot (x - q_1) \\
&\quad + \Xi^\kappa(q_2, p_2) \cdot ((\hat{x} - \delta_x/2) - X^\kappa(q_2, p_2)) - \Xi^\kappa(q_1, p_1) \cdot ((\hat{x} + \delta_x/2) - X^\kappa(q_1, p_1)) \\
&\quad + i\Theta_0^y(y - q_2)^2/2 + i\Theta_0^y(x - q_1)^2/2 \\
&\quad + i\Theta_0^x((\hat{x} - \delta_x/2) - X^\kappa(q_2, p_2))^2/2 + i\Theta_0^x((\hat{x} + \delta_x/2) - X^\kappa(q_1, p_1))^2/2
\end{aligned}
$$

where we used the same transformation as before.

In a first step, we establish decay in w to turn the kernel into an absolutely convergent integral. We have

$$\nabla_{\delta_\xi} \Omega^\kappa = \hat{x} - w.$$

Defining

$$L_{\delta_\xi} = \frac{1 - i\overline{\nabla_{\delta_\xi}\Omega^\kappa} \cdot \nabla_{\delta_\xi}}{1 + \left|\nabla_{\delta_\xi}\Omega^\kappa\right|^2} = \frac{1 + i(\hat{x} - w) \cdot \nabla_{\delta_\xi}}{1 + |\hat{x} - w|^2},$$

we have

$$L_{\delta_\xi} e^{i\Omega^\kappa} = e^{i\Omega^\kappa}$$

and the multinomial theorem gives

$$\left(L_{\delta_\xi}^\dagger\right)^k = \langle \hat{x} - w\rangle^{-2k} \sum_{k_1 + \ldots + k_{d+1} = k} \binom{n}{k_1, \ldots, k_{d+1}} i^{k - k_{d+1}} \prod_{j=1}^d \left((\hat{x} - w)_j \partial_{(\delta_\xi)_j}\right)^{k_j}. \tag{5.14}$$

and hence

$$\left|\left(L_{\delta_\xi}^\dagger\right)^k (u\overline{v})\right| \leq \frac{M_{l_1}^{\delta_\xi}}{\langle \hat{x} - w\rangle^k} \sum_{|\alpha| \leq l_1} \left|\partial_{\delta_\xi}^\alpha (u\overline{v})\right|,$$

which provides enough decay for $k = d + 1$.

Dealing now with an absolutely convergent integral, we are allowed to exchange the order of integration and to transform the integration variable w into $w - \hat{x}$. Doing so, we have

$$
\begin{aligned}
\Im\Omega^\kappa &= \Theta_0^y(x - q_1)^2/2 + \Theta_0^y(y - q_2)^2/2 \\
&\quad + \Theta_0^x\left(\hat{x} - \frac{X^\kappa(q_1, p_1) + X^\kappa(q_2, p_2)}{2}\right)^2 + \Theta_0^x\left(\delta_x - [X^\kappa]_{(q_2,p_2)}^{(q_1,p_1)}\right)^2/4
\end{aligned}
$$

and

$$\begin{pmatrix} \nabla_w \\ \nabla_{\hat{\xi}} \\ \nabla_{\hat{x}} \end{pmatrix} \Omega^\kappa = \begin{pmatrix} -\delta_\xi \\ \delta_x \\ -\left[\Xi^\kappa\right]_{(q_2,p_2)}^{(q_1,p_1)} + 2i\Theta_0^x\left(\hat{x} - \frac{X^\kappa(q_1,p_1) + X^\kappa(q_2,p_2)}{2}\right) \end{pmatrix}.$$

We introduce the operators

$$L_w = \frac{1 - i\overline{\nabla_w \Omega^\kappa} \cdot \nabla_w}{1 + |\nabla_w \Omega^\kappa|^2} = \frac{1 + i\delta_\xi \cdot \nabla_w}{1 + |\delta_\xi|^2}$$

$$L_{\hat{\xi}} = \frac{1 - i\Theta_0^x \overline{\nabla_{\hat{\xi}} \Omega^\kappa} \cdot \nabla_{\hat{\xi}}}{1 + \left|(\Theta_0^x)^{1/2} \nabla_{\hat{\xi}} \Omega^\kappa\right|^2} = \frac{1 - i\Theta_0^x \delta_x \cdot \nabla_{\hat{\xi}}}{1 + \left|(\Theta_0^x)^{1/2} \delta_x\right|^2}$$

$$L_{\hat{x}} = \frac{1 - i\left(\Theta_0^x\right)^{-1} \overline{\nabla_{\hat{x}} \Omega^\kappa} \cdot \nabla_{\hat{x}}}{1 + \left|(\Theta_0^x)^{-\frac{1}{2}} \nabla_{\hat{x}} \Omega^\kappa\right|^2}$$

which fulfill $L_* e^{i\Omega^\kappa} = e^{i\Omega^\kappa}$, where $*$ stands for $w, \hat{\xi}$ or $\hat{x}$. Moreover

$$\left|\left(L_w^\dagger\right)^{l_1}(u\overline{v})\right| \leq \frac{M_{l_1}^{(w)}}{\langle\delta_\xi\rangle^{l_1}} \sum_{|\alpha| \leq l_1} |\partial_w^\alpha (u\overline{v})|$$

$$\left|\left(L_{\hat{\xi}}^\dagger\right)^{l_2}(u\overline{v})\right| \leq \frac{M_{l_2}^{(\hat{\xi})}}{\left\langle(\Theta_0^x)^{1/2} \delta_x\right\rangle^{l_2}} \sum_{|\alpha| \leq l_2} \left|\left((\Theta_0^x)^{1/2} \partial_{\hat{\xi}}\right)^\alpha (u\overline{v})\right|$$

$$\left|\left(L_{\hat{x}}^\dagger\right)^{l_3}(u\overline{v})\right| \leq \frac{M_{l_3}^{(\hat{x})}}{\left\langle(\Theta_0^x)^{-1/2} \left[\Xi^\kappa\right]_{(q_2,p_2)}^{(q_1,p_1)}\right\rangle^{l_3}} \sum_{|\alpha| \leq l_3} \left|\left((\Theta_0^x)^{-1/2} \nabla_{\hat{x}}\right)^\alpha (u\overline{v})\right|$$

and

$$\begin{aligned}
&\left|\left(L_w^\dagger\right)^{l_1}\left(L_{\hat{\xi}}^\dagger\right)^{l_2}\left(L_{\hat{x}}^\dagger\right)^{l_3}(u\overline{v})\right| \\
&\leq M_{l_1}^{(w)} M_{l_2}^{(\hat{\xi})} M_{l_3}^{(\hat{x})} \sum_{\alpha_1 \leq l_1} \sum_{\alpha_2 \leq l_2} \sum_{\alpha_3 \leq l_3} \left\|(\Theta^x)^{\frac{1}{2}}\right\|^{|\alpha_2|} (\lambda^x)^{-\frac{|\alpha_3|}{2}} \left|\partial_w^{\alpha_1} \partial_{\hat{\xi}}^{\alpha_2} \partial_{\hat{x}}^{\alpha_3} (u\overline{v})\right| \\
&\qquad \times \langle\delta_\xi\rangle^{-l_1} \left\langle(\Theta_0^x)^{1/2} \delta_x\right\rangle^{-l_2} \left\langle(\Theta_0^x)^{-1/2} \left[\Xi^\kappa\right]_{(q_2,p_2)}^{(q_1,p_1)}\right\rangle^{-l_3}
\end{aligned}$$

by Lemma 10.2. Taking the explicit form of $\left(L_{\delta_\xi}\right)^{d+1}$ given in (5.14) into account, we have

$$\begin{aligned}
&|K(x,y)| \\
&= \left|\int_{\mathbb{R}^{9d}} e^{i\Omega^\kappa} \left(L_w^\dagger\right)^{l_1}\left(L_{\hat{\xi}}^\dagger\right)^{l_2}\left(L_{\hat{x}}^\dagger\right)^{l_3}\left(L_{\delta_\xi}^\dagger\right)^{d+1}(u\overline{v})\; dq_1\, dq_2\, dp_1\, dp_2\, dx_1'\, dx_2'\, d\xi_1\, d\xi_2\, dw\right| \\
&\leq C_{l_1,l_2,l_3} \\
&\quad \int_{\mathbb{R}^{9d}} \langle\delta_\xi\rangle^{-l_1} \left\langle(\Theta_0^x)^{\frac{1}{2}} \delta_x\right\rangle^{-l_2} \left\langle(\Theta_0^x)^{-1/2} \left[\Xi^\kappa\right]_{(q_2,p_2)}^{(q_1,p_1)}\right\rangle^{-l_3} \langle w\rangle^{-(d+1)} \\
&\qquad e^{-\Theta_0^y (y-q_2)^2/2} e^{-\Theta_0^y (x-q_1)^2/2} e^{-\Theta_0^x \left(\hat{x} - \frac{X^\kappa(q_1,p_1)+X^\kappa(q_2,p_2)}{2}\right)^2} e^{-\Theta_0^x \left(\left[X^\kappa\right]_{(q_2,p_2)}^{(q_1,p_1)} - \delta_x\right)^2/4} \\
&\qquad \sum_{\substack{\alpha_1 \leq l_1, \alpha_2 \leq l_2 \\ \alpha_3 \leq l_3, \alpha_4 \leq d+1}} \left\|(\Theta^x)^{\frac{1}{2}}\right\|^{|\alpha_2|} (\lambda^x)^{-\frac{|\alpha_3|}{2}} \left|\partial_w^{\alpha_1} \partial_{\hat{\xi}}^{\alpha_2} \partial_{\hat{x}}^{\alpha_3} \partial_{\delta_\xi}^{\alpha_4} (u\overline{v})\right| \; dq_1\, dq_2\, dp_1\, dp_2\, d\hat{x}\, d\delta_x\, d\hat{\xi}\, d\delta_\xi\, dw\, dy.
\end{aligned}$$

Performing the y, w and $\hat{x}$-integrals, we can estimate

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^d}\int |K(x,y)|\ dy \\
&\leq C_{l_1,l_2,l_3}\left\|\langle w\rangle^{-(d+1)}\right\|_{L^1(\mathbb{R}^d)}\left\|e^{-\Theta_0^x\hat{x}^2/2}\right\|_{L^1(\mathbb{R}^d)}\left\|e^{-\Theta_0^y y^2/2}\right\|_{L^1(\mathbb{R}^d)} \\
&\int_{\mathbb{R}^{7d}}\langle\delta_\xi\rangle^{-l_1}\left\langle(\Theta_0^x)^{\frac12}\,\delta_x\right\rangle^{-l_2} e^{-\Theta_0^x\left([X^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}-\delta_x\right)^2/4}\left\langle(\Theta_0^x)^{-\frac12}[\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right\rangle^{-l_3} \\
&\qquad\sum_{\alpha_1\leq l_1\alpha_2\leq l_2\alpha_3\leq l_3\alpha_4\leq d+1}\left\|(\Theta^x)^{\frac12}\right\|^{|\alpha_2|}(\lambda^x)^{-\frac{|\alpha_3|}{2}}\left|\partial_w^{\alpha_1}\partial_{\hat{\xi}}^{\alpha_2}\partial_{\hat{x}}^{\alpha_3}\partial_{\delta_\xi}^{\alpha_4}(u\overline{v})\right|\ dq_1\,dq_2\,dp_1\,dp_2\,d\delta_x\,d\hat{\xi}\,d\delta_\xi
\end{aligned}$$

and literally the same estimate for $\sup_{y\in\mathbb{R}^d}\int |K(x,y)|\ dx$.

To get the decay in $\delta(K_u,K_v)$, we split the δ_x-integral into the two regions

1. $K_> := \{\delta_x : 2\,|\delta_x| > |(X^\kappa(q_1,p_1) - X^\kappa(q_2,p_2))|\}\subset\mathbb{R}^d$ and
2. $K_\leq := \{\delta_x : 2\,|\delta_x| \leq |(X^\kappa(q_1,p_1) - X^\kappa(q_2,p_2))|\}\subset\mathbb{R}^d$,

where we suppressed the dependence of the sets on the phase-space variables in the notation. Now the elements of $K_\leq$ fulfill

$$|(X^\kappa(q_1,p_1) - X^\kappa(q_2,p_2)) - \delta_x| \geq \left|\frac{X^\kappa(q_1,p_1) - X^\kappa(q_2,p_2)}{2}\right|,$$

and we get

$$\begin{aligned}
&\sup_{x\in\mathbb{R}^d}\int |K(x,y)|\ dy \\
&\leq C_{l_1,l_2,l_3}\left(\det\Theta_0^x\det\Theta_0^y\right)^{-1/2}\int\langle\delta_\xi\rangle^{-l_1}\left\langle(\Theta_0^x)^{-\frac12}\,[\Xi^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right\rangle^{-l_3} \\
&\quad\left(\int_{K_\leq} e^{-\Theta_0^x\left([X^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}\right)^2/4}\left\langle(\Theta_0^x)^{\frac12}\,\delta_x\right\rangle^{-l_2} d\delta_x\right. \\
&\qquad\left.+\int_{K_>}\left\langle(\Theta_0^x)^{\frac12}\,[X^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}/2\right\rangle^{-l_2} e^{-\Theta_0^x\left([X^\kappa]^{(q_1,p_1)}_{(q_2,p_2)}-\delta_x\right)^2/4}d\delta_x\right) \\
&\quad\sum_{\alpha_1\leq l_1\alpha_2\leq l_2\alpha_3\leq l_3\alpha_4\leq d+1}\left\|(\Theta^x)^{\frac12}\right\|^{|\alpha_2|}(\lambda^x)^{-\frac{|\alpha_3|}{2}}\left|\partial_w^{\alpha_1}\partial_{\hat{\xi}}^{\alpha_2}\partial_{\hat{x}}^{\alpha_3}\partial_{\delta_\xi}^{\alpha_4}(u\overline{v})\right|\ dq_1\,dq_2\,dp_1\,dp_2\,d\hat{\xi}\,d\delta_\xi \\
&\leq C_{l_1,l_2,l_3}\left(\det\Theta_0^x\right)^{-1}\left(\det\Theta_0^y\right)^{-1/2}\left\langle\delta_{\Theta_0^x}(K_u,K_v)\right\rangle^{-\min(l_2,l_3)}\left\langle\delta(K_u',K_v')\right\rangle^{-l_1} \\
&\quad\max\left(\left\|\langle x\rangle^{l_4}\,e^{-x^2/16}\right\|_{L^\infty(\mathbb{R}^d)}\left\|\langle\delta_x\rangle^{-l_3}\right\|_{L^1(\mathbb{R}^d)},\left\|e^{-\delta_x^2/2}\right\|_{L^1(\mathbb{R}^d)}\right) \\
&\int\sum_{\alpha_1\leq l_1\alpha_2\leq l_2\alpha_3\leq l_3\alpha_4\leq d+1}\left\|(\Theta^x)^{\frac12}\right\|^{|\alpha_2|}(\lambda^x)^{-\frac{|\alpha_3|}{2}}\left|\partial_w^{\alpha_1}\partial_{\hat{\xi}}^{\alpha_2}\partial_{\hat{x}}^{\alpha_3}\partial_{\delta_\xi}^{\alpha_4}(u\overline{v})\right|\ dq_1\,dq_2\,dp_1\,dp_2\,d\hat{\xi}\,d\delta\xi
\end{aligned}$$

and exactly the same estimate for $\sup_{y\in\mathbb{R}^d}\int |K(x,y)|\ dx$. Thus the Schur Lemma gives (5.11).

□

Proof of Theorem 5.4

Proof of Theorem 5.4. We remind the reader that it is enough to prove the result for $\varepsilon = 1$ and $\Theta_0^x, \Theta_0^y \in \mathcal{C}_{\text{const}}$. The strategy of the proof is exactly the same as in the one of Theorem 4.11. We introduce the partition of unity $\{\chi_{\Gamma'}\}_{\Gamma' \in \mathbb{Z}^d}$, which is the d-dimensional analogue of the partition of unity $\{\chi_\Gamma\}_{\Gamma \in \mathbb{Z}^{2d}}$ already used in the proof of Theorem 4.11.

We define the symbols $u_{\Gamma\Gamma'}$ by $u_{\Gamma\Gamma'}(x, \xi, x', y, q, p) := \chi_\Gamma(q, p)\chi_{\Gamma'}(\xi)u(x, \xi, x', y, q, p)$, which are supported in $\mathbb{R}^d \times [K' + \Gamma'] \times \mathbb{R}^{2d} \times [K + \Gamma]$. Proposition 5.9 shows that

$$\left\| \mathcal{R}^1\Big(\kappa; u_{\Gamma_1\Gamma_1'}; \Theta_0^x, \Theta_0^y\Big)\, \mathcal{R}^1\Big(\kappa; u_{\Gamma_2\Gamma_2'}; \Theta_0^x, \Theta_0^y\Big)^* \right\| + \left\| \mathcal{R}^1\Big(\kappa; u_{\Gamma_1\Gamma_1'}; \Theta_0^x, \Theta_0^y\Big)^* \mathcal{R}^1\Big(\kappa; u_{\Gamma_2\Gamma_2'}; \Theta_0^x, \Theta_0^y\Big) \right\|$$

is dominated by

$$\begin{aligned} &\omega(\Gamma_1 - \Gamma_2, \Gamma_1' - \Gamma_2') \\ :=\ & \frac{C_{l_1,l_2}[M_0^\kappa; \Theta^x; \Theta^y]}{\Big(1 + \eta^2_{[\kappa;\Theta_0^x,\Theta_0^y]} \left|\Gamma_1 - \Gamma_2\right|_\infty^2\Big)^{l_1/2} \Big(1 + \left|\Gamma_1' - \Gamma_2'\right|_\infty^2\Big)^{l_2/2}} \max_{\substack{|\alpha| \le l_1 + l_2 \\ |\beta| \le \max(l_1, l_2) \\ |\gamma| \le l_1 + d + 1}} \left\| \partial^\alpha_{(x,y)} \partial^\beta_{x'} \partial^\gamma_\xi u \right\|_{L^\infty(\mathbb{R}^{6d})} \end{aligned}$$

where $\eta_{[\kappa;\Theta_0^x,\Theta_0^y]} = \min\Big(c_{\Lambda[\Theta_0^x]\circ\kappa}, c_{\Lambda[\Theta_0^y]}\Big)$. As in the proof of Theorem 4.11, we have to assure the convergence of the series

$$\begin{aligned} &\left[C_{l_1,l_2}[M_0^\kappa; \Theta^x; \Theta^y] \max_{\substack{|\alpha| \le l_1 + l_2 \\ |\beta| \le \max(l_1, l_2) \\ |\gamma| \le l1 + d + 1}} \left\| \partial^\alpha_{(x,y)} \partial^\beta_{x'} \partial^\gamma_\xi u \right\|_{L^\infty(\mathbb{R}^{6d})} \right]^{-1} \sum_{\substack{\Gamma \in \mathbb{Z}^{2d} \\ \Gamma' \in \mathbb{Z}^d}} \sqrt{\omega(\Gamma, \Gamma')} \\ \le\ & C \left[\sum_{k_1 \ge 2} \frac{k_1^{2d-1}}{\Big(1 + \eta^2_{[\kappa;\Theta_0^x,\Theta_0^y]} k_1^2\Big)^{l_1/4}} \right] \left[\sum_{k_2 \ge 2} \frac{k_2^{d-1}}{\big(1 + k_2^2\big)^{l_2/4}} \right]. \end{aligned}$$

and have thus to fulfill

$$l_1/2 - (2d - 1) > 1 \text{ and } l_2/2 - (d - 1) > 1.$$

Hence, the smallest integers l_1 and l_2 we can choose are $l_1 = 4d + 1$ and $l_2 = 2d + 1$. The Cotlar-Stein Lemma shows that the series

$$\sum_\Gamma \mathcal{R}^1(\kappa; u_\Gamma; \Theta_0^x, \Theta_0^y)$$

is strongly convergent to a bounded operator whose norm is dominated by (5.4). The same argument as in the proof of Theorem 4.11 shows that the operator-limit coincides with the Fourier Integral Operator defined before. □

Part III

Initial Value Representations

6 Prior approximation results on the propagator

Before we continue on our way to the main result, we discuss related work both in the mathematical and chemical literature.

6.1 The origin of Initial Value Representations

We give a short history of IVRs. Due to the overwhelming amount of papers in the chemical literature, we restrict the discussion to two issues here and refer the reader who is interested in a complete overview of the field to the review articles [Mil01], [TW04] and [Kay07]. The first aspect we want to address is why the class of methods was baptised Initial Value Representations, i.e. why there is so much emphasis on the type of problems one has to solve to obtain the approximation. Second, we want to sketch the developments, which led to the specific form of the operators $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$.

The first semiclassical expression goes back to [VV28] and [Gut67]. This van-Vleck propagator approximates the Schwartz-kernel $K^{(t,s)}(x,y) \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ of the unitary propagator $U(t,s)$ of (1.8) by the expression

$$K^{(t,s)}(x,y) \approx \frac{1}{(2\pi i\varepsilon)^{d/2}} \sum_{p_j | X^{\kappa^{(t,s)}}(y,p_j)=x} \left|\det X_p^{\kappa^{(t,s)}}(y,p_j)\right|^{-\frac{1}{2}} e^{\frac{i}{\varepsilon}S^{\kappa^{(t,s)}}(y,p_j) - i\pi\nu_j/2}, \tag{6.1}$$

which is closely related to the Maslov canonical operator of Section 3.1. The manifold which corresponds to $\mathcal{L}_S$ is derived from the delta distribution $\delta(y)$: writing

$$\psi_0(y) = (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot y} \left(\mathcal{F}^\varepsilon\psi_0\right)(\xi)\, d\xi$$

one has formally

$$\psi(t,x) = (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} \left(U(t,s)e^{\frac{i}{\varepsilon}\xi\cdot}\right)(x) \left(\mathcal{F}^\varepsilon\psi_0\right)(\xi)\, dx.$$

Now the plane wave $\xi \mapsto e^{\frac{i}{\varepsilon}\xi\cdot y}$ looks like an WKB-initial datum, which is associated to the manifold

$$\mathcal{L}_y = \left\{(y,p)\middle| p \in \mathbb{R}^d\right\}$$

and one can use the Maslov formalism to get (6.1).

There are several papers in the mathematical literature, which give a rigorous sense to the van-Vleck expression. First, there is [Fuj75] which discusses L^2-boundedness properties of the operator with the kernel (6.1) in the case where there is only one contributing trajectory. Later on in [Fuj79] these results are used to justify the time-slicing approach to Feynman's path-integrals in terms of the van-Vleck propagator. [Yaj79] uses Fujiwara's result to derive a semiclassical approximation to certain scattering problems. Finally there are [Rob88], where a van-Vleck-type expression is used to describe the time-evolution of coherent states and [BR01], where L^2-operator norm results for the van-Vleck expression are shown.

From a practical point of view (6.1) has two drawbacks. The first one is connected to the caustic problem, which becomes manifest in the points for which $\det X_q^{\kappa^{(t,s)}}(y, p_j) = 0$ and leads to a division by zero. Principally, this problem can be circumvented by the Hörmander-Maslov theory, but the local change of coordinates in phase-space seems not feasible for a computational approach. (6.1) contains a second difficulty: to identify the momenta, which contribute to the sum, one has to solve the boundary-value problem

$$\text{Given } x, y \in \mathbb{R}^d, \text{ find } p \text{ such that } X^{\kappa^t}(y,p) = x,$$

which is a serious challenge especially in high dimensions.

The "basic IVR trick" solves those difficulties at the expense of another computationally hard problem, namely the discretization of an oscillatory integral. It appears for the first time in [Mil70], where the S-matrix of scattering theory is studied in semiclassical approximation. As we do not want to discuss the specifics of this theory, we follow the presentation of [Kay07], which explains the principal approach in the case of the integral kernel of $U(t,s)$ and allows to connect with (6.1). First, one adds the identity on both sides of the kernel in terms of δ-distributions, i.e.

$$K^{(t,s)}(x,y) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \delta(x-q_t)K^{(t,s)}(q_t,q)\delta(y-q)\, dq_t\, dq. \tag{6.2}$$

Now one uses (6.1) to obtain a semiclassical approximation of $K(t,s)$ and performs the change of variable $q_t \to p$, where q_t is considered as $q_t = \kappa^{(t,s)}(q,p)$. One obtains

$$\begin{aligned} K^{(t,s)}(x,y) &\approx (2\pi i\varepsilon)^{-d/2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \delta(x-q_t)\left|\det(X_p^{\kappa^{(t,s)}}(q,p))\right|^{\frac{1}{2}} e^{\frac{i}{\varepsilon}S^{\kappa^{(t,s)}}(q,p)-i\pi\nu/2}\delta(y-q)\, dq\, dp \\ &= (2\pi i\varepsilon)^{-d/2}\int_{\mathbb{R}^d} \delta(x-q_t)\left|\det(X_p^{\kappa^{(t,s)}}(q,p))\right|^{\frac{1}{2}} e^{\frac{i}{\varepsilon}S^{\kappa^{(t,s)}}(q,p)-i\pi\nu/2}\, dp. \end{aligned}$$

Now the boundary value problem has been transformed into the solution of initial value problems. Moreover, the prefactor in this expression is well-behaved compared to the one in (6.1). However, considering the decay of the p-integral and recalling the discussion about Hörmander-Maslov theory, it is clear that the caustic problem is still implicitly present in the phase function.

Heller approached semiclassical approximations from a different direction. In [Hel75b] the time-evolution of coherent states $g^\varepsilon_{(q,p)}$ is studied and the approximate expression (0.6) for the propagation of coherent states is formally derived. Later on in [Hel75a] it is observed that one gets a reasonable approximation, if one expands an arbitrary initial datum into coherent states and moves each Gaussian along the classical flow without the time-dependent spreading of the full approximation, i.e.

$$\begin{aligned} U(t,s)\varphi(x) &\approx (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} g^\varepsilon_{\kappa^{(t,s)}(q,p)}\left\langle g^\varepsilon_{(q,p)}\middle|\varphi\right\rangle_{L^2(\mathbb{R}^d)}\, dq\, dp \\ &= \left(\mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; 2^{d/2}; \mathrm{id}, \mathrm{id}\right)\varphi\right)(x). \end{aligned}$$

A byproduct of the proof of our main theorem is that this “Frozen Gausian IVR” is an approximation to the propagator for short times in the sense that

$$\left\| U(t,s) - \left(\mathcal{I}^{\varepsilon}\left(\kappa^{(t,s)}; 2^{d/2}; \mathrm{id}, \mathrm{id}\right)\varphi\right)(x)\right\|_{L^2\to L^2} \leq C\varepsilon$$

if $|t-s| \leq \varepsilon T$.

The symbol, which turns this expression into an approximation for longer times is established in [HK84] and [KHL86] and is known as the Herman-Kluk prefactor

$$u_{\mathrm{HK}}(t,s,q,p) = \left[\det\left(X_q^{\kappa^{(t,s)}}(q,p) - iX_p^{\kappa^{(t,s)}}(q,p) + i\Xi_q^{\kappa^{(t,s)}}(q,p) + \Xi_p^{\kappa^{(t,s)}}(q,p)\right)\right]^{\frac{1}{2}},$$

where the square root is chosen by continuity in time. The original derivation shows some similarity to Millers IVR argument. As in (6.2), Herman and Kluk add the identity on both sides of the kernel but instead of δ-distributions, the “overcomplete basis of coherent states” is used. After the insertion of the van-Vleck expression, the integration variables are transformed and a stationary phase approximation in performed. Due to the carefree use of complex variables during this process the original derivation is not beyond doubt even in the chemical literature, compare [BdAK$^+$01] and [Kay06].

There are three additional derivations of the Herman-Kluk expression. First, in [Kay94] the general form of IVRs is investigated. It is observed that $\mathcal{I}^{\varepsilon}(\kappa; u; \Theta^x, \Theta^y)$ reduces to the van-Vleck propagator in the limit $\varepsilon \to 0$ for any choice of Θ^x and Θ^y, if the correct symbol is used. In particular it is shown that the Herman-Kluk prefactor is the correct choice for $\Theta^x, \Theta^y \in \mathcal{C}_{\mathrm{const}}$. Second, there is the derivation of Miller [Mil02], which was refined in [DE06]. Here, the “overcomplete basis of coherent states” is added on both sides of an operator of the form $\mathcal{I}^{\varepsilon}\big(\kappa^{(t,s)}; u; \mathrm{id}, \mathrm{id}\big)$ and an equation for u is deduced with help of a stationary phase argument. Finally, there is the derivation of Kay in [Kay06] which is the most satisfactory from a mathematical point of view, as the author establishes on a formal level that the Herman-Kluk expression is an asymptotic solution to (1.8). The composition results in this section add the necessary rigor to those arguments.

[Kay06] was written in response to a debate on the Herman-Kluk propagator, which was started by [BdAK$^+$01]. There the authors claimed that the Herman-Kluk propagator is not a valid semiclassical expression. This conclusion was drawn on the basis of a fundamental misunderstanding of the Herman-Kluk propagator, as the authors did not realize that the phase space integral is a fundamental component of the operator. Instead they assumed that Herman and Kluk claimed

$$\left(U(t,s)g^{\varepsilon}_{(q,p)}\right)(x) \approx u_{\mathrm{HK}}(t,s,q,p)\, g^{\varepsilon}_{\kappa^{(t,s)}(q,p)}(x).$$

Despite the questionable criticism of Baranger et al. the paper proved to be fruitful in two aspects. Besides the work of Kay, it entailed a series of papers, in which the relation between semiclassical propagators and PDOs with smoothed Weyl symbol are studied. Considering that Initial Value Representations are aimed at high-dimensional problems, and that the potential might even arise from electronic structure calculations, the author wants to express his doubts about the practical relevance of this approach.

6.2 Fourier Integral Operators as approximate propagators

Whereas the approximations derived in the chemical literature are constructed with their computational usefulness in mind, mathematicians are traditionally more interested in a conceptional understanding of the problem. Hence, many approximations derived in the mathematical community are not feasible for an implementation.

This applies for example to the works [KKG81] and [Kit82]. There, the propagator of (1.8) is expressed by FIOs with real phase. The main technical problem is again related to the caustics. The authors require that the the mappings

$$\begin{aligned} q : \mathbb{R}^d &\to \mathbb{R}^d & \qquad p : \mathbb{R}^d &\to \mathbb{R}^d \\ x &\mapsto q(t,s,x,p) & \qquad \xi &\mapsto p(t,s,q,\xi), \end{aligned} \tag{6.3}$$

are diffeomorphisms, where q, p, x and ξ are related by

$$(x,\xi) = \kappa^{(t,s)}(q,p).$$

More prosaically speaking, this conditions means that the boundary value problems

Find the initial position, when initial momentum and final position are given

and

Find the initial momentum, when final momentum and initial position are given

have unique solutions with good dependence on their parameters.

If this condition is fulfilled, one can define the operator

$$\left[\mathcal{I}^{\varepsilon}_{\mathrm{KKG}}\left(\kappa^{(t,s)};u\right)\varphi\right](x) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\Phi^{\kappa^{(t,s)}}_{\mathrm{KGG}}(x,y,p)}u(t,s,x,p)\varphi(y)\,dp\,dy$$

with phase function

$$\Phi^{\kappa^{(t,s)}}_{\mathrm{KKG}}(x,y,p) = S^{\kappa^{(t,s)}}(q(t,s,x,p),p) + p\cdot(y - q(t,s,x,p))$$

and symbol $u \in S[\infty;2d]$. Unter the assumption of Schrödinger operators with subquadratic potentials, the main result of [KKG81] is that the propagator of (1.8) may for sufficiently large N be expressed as

$$U(t,s) = \prod_{n=1}^{N} \mathcal{I}^{\varepsilon}_{\mathrm{KKG}}\left(\kappa^{(t_n,t_{n-1})};u\right),$$

where

$$t_n = s + \frac{n}{N}(t-s), \qquad n = 0,\dots,N$$

and the symbol u arises from transport equations related to the transport equation of the WKB-methodology (3.2). In [Kit82] it is shown that the expression holds with $N = 1$ under suitable assumptions on the potential and sufficiently large times, see below.

As a corollary, the authors establish the following semiclassical approximation results for the propagator:

6.1 Theorem. *Let $h(t,x,\xi) = \xi^2/2 + V(t,x)$.*

[KKG81] *If h is subquadratic, there is $T_0 > 0$ and a family of symbols $u_n, n \leq N$ such that*

$$\left\| U(t,s) - \mathcal{I}^\varepsilon_{\mathrm{KKG}}\left(\kappa^{(t,s)}; \sum_{n=0}^{N} \varepsilon^n u_n\right)\right\|_{L^2\to L^2} \leq C\varepsilon^{N+1}$$

for all (t,s) with $|t-s| < T_0$.

[Kit82] *If there is $\delta > 0$ such that $|\partial_x^\alpha V(t,x)| \leq C\langle t\rangle^{-(\delta+|\alpha|)}$ uniformly in x for all $|\alpha| \geq 1$, there is $T_0 > 0$ and a family of symbols $u_k, k \leq N$ such that*

$$\left\| U(t,s) - \mathcal{I}^\varepsilon_{\mathrm{KKG}}\left(\kappa^{(t,s)}; \sum_{n=0}^{N} \varepsilon^n u_n\right)\right\|_{L^2\to L^2} \leq C\varepsilon^{N+1}$$

for all (t,s) with $T_0 \leq s \leq t$.

Obviously, the strong assumptions on the time-intervals and the potentials are a tribute to the caustic problem. Its general avoidance of is the major advantage of complex-valued phase functions. Surprisingly, the mathematical literature on semiclassical FIOs with complex phase is relatively sparse.

The first works which discuss such operators in the context of Schrödinger equations are [LS00] and [But02]. These authors essentially impose the following restrictions on $\mathrm{op}^\varepsilon(h)$

1. There is $m \in \mathbb{N}$ such that $h \in S[m;2d]$.
2. There is $\varepsilon_0 > 0$ such that $\mathrm{op}^\varepsilon(h)$ is essentially self-adjoint for all $\varepsilon \leq \varepsilon_0$.

The operators used in [LS00] and [But02] are of the form

$$\left(\mathcal{I}^\varepsilon_{\mathrm{LS}}(\kappa;u)\psi\right)(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon}\Phi^\kappa_{\mathrm{LS}}(x,y,p;\Theta)} u(t,y,p)\psi(y)\, dp\, dy,$$

where the phase function $\Phi^{\kappa^{(t,s)}}_{\mathrm{LS}}$ is given by

$$\Phi^\kappa_{\mathrm{LS}}(x,y,p;\Theta) = S^{\kappa^{(t,s)}}(y,p) + \Xi^\kappa(y,p)\cdot(x - X^\kappa(y,p)) + i\Theta(x - X^\kappa(y,p))^2/2$$

for $\Theta \in \mathcal{C}_{\mathrm{const}}$ and the symbol u is compactly supported. In particular, the kernel involves only an integration over momentum space compared to the phase-space integral used in the definition of $\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)$. With these assumptions, the results are

6.2 Theorem. *Let $U(t,s)$ be the propagator associated to* (1.8)*, where the symbol h fulfills the assumptions discussed before.*

[LS00] *Let $\chi \in C_0^\infty(\Omega)$, where $\Omega \subset \mathbb{R}^{2d}$ is a bounded subset of the phase space. There is a constant $C(h,\Omega,T_0)$ such that for any $N \in \mathbb{N}$, there are symbols $u_k \in C_0^\infty(\Omega)$, $k \leq N$ such that*

$$\left\| \left[U(t,s) - \mathcal{I}^\varepsilon_{\mathrm{LS}}\left(\kappa^t; \sum_{k=0}^{N} \varepsilon^k u_k\right)\right]\mathrm{op}^\varepsilon(\chi)\right\|_{L^2\to L^2} \leq C(h,\Omega,T_0)\varepsilon^{N+1-d}.$$

[But02] *Let $\chi_1, \chi_2 \in C_0^\infty(\Omega)$, where $\Omega \subset \mathbb{R}^{2d}$ is a bounded subset of the phase space. For any $N \in \mathbb{N}$, there are symbols $u_k \in C_0^\infty(\Omega)$, $k \leq N$ such that*

$$\left\| \operatorname{op}^\varepsilon(\chi_1) \left[U(t,s) - \mathcal{I}_{\mathrm{LS}}^\varepsilon \left(\kappa^t; \sum_{k=0}^N \varepsilon^k u_k \right) \right] \operatorname{op}^\varepsilon(\chi_2) \right\|_{L^2 \to L^2} \leq C_N(h, \chi_1, \chi_2, \Theta) \varepsilon^{N+1}.$$

Obviously, the results are closely related. In fact, [But02] was written to overcome a flaw in the proof of [LS00] which forced the symbol h to be analytic in ξ. A second improvement concerns the error bound, which is dimension independent in the latter result. As no explicit explanation for this is given in [But02], we refer the reader to Proposition 5 of [RS08], where a similar bound is established.

The Thawed-Gaussian IVR $\mathcal{I}^\varepsilon\big(\kappa^{(t,s)}; u_{\mathrm{TGA}}; \Theta_{\mathrm{TGA}}, \mathrm{id}\big)$ with

$$\Theta_{\mathrm{TGA}}(t,s,q,p) = -i \left(X_q^{\kappa^{(t,s)}} + i X_p^{\kappa^{(t,s)}} \right)^{-1} \left(\Xi_q^{\kappa^{(t,s)}} + i \Xi_p^{\kappa^{(t,s)}} \right) \quad \text{and} \tag{6.4}$$

$$u_{\mathrm{TGA}}(t,s,q,p) = 2^{d/2} \left(\det \left(X_q^{\kappa^{(t,s)}} + i X_p^{\kappa^{(t,s)}} \right)^{-1} \right)^{1/2} \tag{6.5}$$

has been discussed earlier in [BR01]. Under similar assumption on h as in [LS00] the central result reads

6.3 Theorem ([BR01]). *Let $\chi \in C_0^\infty(\mathbb{R}^d)$ and h as discussed before. For every $N \in \mathbb{N}$, there are symbols $u_k \in S[0; 3d]$ depending on q, p and $\left(x - X^{\kappa^{(t,s)}}(q,p)\right)$, which are compactly supported with respect to p such that*

$$\left\| \left[U(t,s) - \mathcal{I}^\varepsilon \left(\kappa^{(t,s)}; \sum_{k=0}^N \varepsilon^{k/2} u_k; \Theta_{\mathrm{TGA}}, \mathrm{id} \right) \right] \chi(-i\varepsilon\nabla_x) \right\| \leq \varepsilon^{N+1/2}.$$

In particular, $u_0 = u_{\mathrm{TGA}}$.

Our result differs in several aspects form the one of Bily and Robert. First, we have to make a stronger assumption on the symbols of $\operatorname{op}^\varepsilon(h)$, namely subquadraticity. On the other hand, this restriction enables us to get rid of the momentum cutoff. Moreover, we show that the TGA expression actually allows for an expansion in whole powers of ε compared to the half-power expansion of [BR01], which is directly inherited from results on the approximate evolution of coherent states.

Finally, we want to mention [Tat04]. Though this work is not semiclassical, it is in some sense very close to our presentation. There, a class of operators containing $\mathcal{I}^1(\kappa; u; \mathrm{id}, \mathrm{id})$ is discussed. In particular, it is shown that under the assumption of subquadratic symbols $h \in S[2; 2d]$, $\mathcal{I}^1\big(\kappa; 2^{d/2}; \mathrm{id}, \mathrm{id}\big)$ is a parametrix for the time-dependent Schrödinger equation (1.8).

7 On the way to an asymptotic solution

The standard approach in asymptotic analysis is a two-step procedure: first, one constructs an asymptotic solution

7.1 Definition. *Let $h^\varepsilon \in S[2;2d]$ be a subquadratic symbol. A family of bounded operators $U_N(t,s)$ is called an* ***asymptotic propagator*** *of order N of the time-dependent Schrödinger equation* (1.8) *if it leaves $\mathcal{S}(\mathbb{R}^d)$ invariant and if there is a family of bounded operators $R_N^\varepsilon(t,s) \in \mathcal{B}(L^2(\mathbb{R}^d))$ such that*

$$\left(i\varepsilon\frac{d}{dt} - \mathrm{op}^\varepsilon(h^\varepsilon(t))\right) U_N(t,s)\psi = R_N^\varepsilon(t,s)\psi, \qquad U(s,s) = \mathrm{id}$$

for all $\psi \in \mathcal{S}(\mathbb{R}^d)$, where

$$\|R_N^\varepsilon(t,s)\|_{L^2\to L^2} \leq C(t,s)\varepsilon^N. \tag{7.1}$$

In the second step, the asymptotic solution is turned into an approximate solution with help of the "Magic Lemma":

7.2 Lemma. *Let $U^\varepsilon(t,s)$ be the propagator of* (1.8) *and $U_N^\varepsilon(t,s)$ an approximate propagator of order $N+1$. We have*

$$\|U_N^\varepsilon(t,s) - U^\varepsilon(t,s)\|_{L^2\to L^2} \leq C(t,s)\varepsilon^N,$$

where

$$C(t,s) = \varepsilon^{-(N+1)}\left|\int_s^t \|R_N^\varepsilon(\tau,s)\|_{L^2\to L^2}\, d\tau\right|.$$

Proof. Let $\psi \in \mathcal{S}(\mathbb{R}^d)$. Using properties of the propagator $U(t,s)$, we have

$$\begin{aligned}
&\|U_N(t,s)\psi - U(t,s)\psi\| = \|U(s,t)U_N(t,s)\psi - \psi\| \\
&= \varepsilon^{-1}\left\|\int_s^t i\varepsilon\frac{d}{d\tau}U(s,\tau)U_N(\tau,s)\psi\, d\tau\right\| \\
&= \varepsilon^{-1}\left\|\int_s^t U(s,\tau)\left[i\varepsilon\frac{d}{d\tau} - \mathrm{op}^\varepsilon(h^\varepsilon(\tau))\right]U_N(\tau,s)\psi\, d\tau\right\| \\
&= \varepsilon^{-1}\left\|\int_s^t U(s,\tau)R_N^\varepsilon(\tau,s)\psi\, d\tau\right\| \leq \varepsilon^{-1}\left|\int_s^t \|R_N^\varepsilon(\tau,s)\|\, d\tau\right| \|\psi\|\,.
\end{aligned}$$

□

In particular, one looses one power in ε, when one turns the asymptotic solution into an approximate one. Subsuming the content of the first and the second part, we have established all boundedness results required in the definition of the asymptotic solution and the application of the "Magic Lemma". In this section we will construct families of FIOs such that (7.1) holds.

7.1 Composition with pseudo-differential operators and time-derivatives

As operators from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^d)$, Fourier Integral operators with complex phase may be composed with pseudodifferential operators. When one tries establishes expansions of these compositions in powers of the semiclassical parameter ε, it turns out that the situation of constant $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$ is easier and more satisfactory than the general case.

For constant matrices Θ^x and Θ^y it is possible to give a full asymptotic expansion in x and y independent symbols and to obtain an remainder, which is $O(\varepsilon^{N+1})$ with a reasonable meaning. In the general case, one has an remainder of order $O(\varepsilon^{N+1})$ in the sense that it is bounded as an operator from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$, but for this one has to make strong assumptions on the symbol of the PDO one is composing with. For this reason, we will provide an result, which is focussed on the application and not entirely satisfactory from a conceptional point of view.

The results use two special notations. First, we introduce the following combination of derivatives

$$\partial_z := (\Theta^y(q,p))^{-1}\,\partial_q - i\partial_p, \tag{7.2}$$

which induces the "divergence"

$$\operatorname{div}_z\left(f(q,p)\right) := \sum_{k=1}^{d} (\Theta^y(q,p))^{-1}_{kl}\,\partial_{q_l} f_k(q,p) - i\sum_{k=1}^{d}\partial_{p_k} f_k(q,p)$$

for functions $f \in C^1(\mathbb{R}^{2d})$. Second, we use the matrix $\mathcal{Z}(q,p) \in S[0;2d]$ which is given by

$$\mathcal{Z}(q,p) := (i\,(\Theta^y(y,p))^{-1} \quad \mathrm{id})(F^\kappa(q,p))^\dagger(-i\Theta^x(y,p) \quad \mathrm{id})^\dagger. \tag{7.3}$$

A lemma in the appendix shows that $\mathcal{Z}(q,p)$ is invertible with $\mathcal{Z}^{-1}(q,p) \in S[0;2d]$.

The first composition result reads:

7.3 Proposition (Composition with PDOs)**.** *Let $h \in S[m_h;2d]$, κ a canonical transformation of class $\mathcal{B}$, $u \in S[m_u;2d]$ and $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$. There are $v_n \in S[m_u+m_h;2d]$, $n \in \mathbb{N}$ such that for any $N \in \mathbb{N}$ there is $v^\varepsilon_{N+1} \in S[(m_h, m_u+m_h);(3d,2d)]$ with*

$$\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y) = \mathcal{I}^\varepsilon\left(\kappa;\sum_{n=0}^{N}\varepsilon^n v_n;\Theta^x,\Theta^y\right) + \varepsilon^{N+1}\mathcal{R}^\varepsilon\left(\kappa;v^\varepsilon_{N+1};\Theta^x,\Theta^y\right).$$

The symbols $v_n, n \in \mathbb{N}$ are given as

$$v_n = L_n[h;\kappa;\Theta^x,\Theta^y]u \qquad \text{and} \qquad v^\varepsilon_{N+1} = L^\varepsilon_N[h;\kappa;\Theta^x,\Theta^y]u,$$

where the $L_n[h;\kappa;\Theta^x,\Theta^y]$ and $L^\varepsilon_N[h;\kappa;\Theta^x,\Theta^y]$ are linear differential operators in (q,p) of degree n whose coefficients are rational functions of $\partial^\alpha_{(x,\xi)}h, n \le |\alpha| \le 2n$ and $\partial^\alpha_{(q,p)}F^\kappa, |\alpha| \le n$ and $\partial^\alpha_{(x,\xi)}h, N+1 \le |\alpha| \le 2N+1$ and $\partial^\alpha_{(q,p)}F^\kappa, |\alpha| \le N+1$ respectively. The explicit expressions *for v_0, v_1 and v_2 are*

$$v_0(q,p) = u(q,p)h(\kappa(q,p)) \tag{7.4}$$

$$\begin{aligned} v_1(q,p) = &-\mathrm{div}_z\left(\left((h_x + i\Theta^x h_\xi)\circ\kappa\right)^\dagger(q,p)\mathcal{Z}^{-1}(q,p)u(q,p)\right) \\ &+ u\frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z((h_x + i\Theta^x h_\xi)\circ\kappa)(q,p)\right) \end{aligned} \tag{7.5}$$

and

$$\begin{aligned} v_2(q,p) = &L_2[h_{\geq 3};\kappa;\Theta^x,\Theta^y]u(q,p) \\ &+ \frac{1}{2}\sum_{k=1}^{d}\mathrm{div}_z\left(u(q,p)\partial_{z_k}\left[((\partial_x + i\Theta^x\partial_\xi)^2 h)\circ\kappa\mathcal{Z}^{-1}(q,p)e_k)\right]^\dagger\mathcal{Z}^{-1}(q,p)\right), \end{aligned} \tag{7.6}$$

where the coefficients of $L_2[h_{\geq 3};\kappa;\Theta^x,\Theta^y]$ on derivatives of h of order 3 and 4.

From the explicit expressions, it is not obvious that the coefficients are rational functions of $\partial^\alpha F^\kappa(q,p)$. This follows from the expression of $\mathcal{Z}^{-1}(q,p)$ via the formula of minors, compare the appendix. The precise form of the differential operators, which can be read of the proof, yields the following corollary:

7.4 Corollary. *Consider the situation of Proposition 7.3.*

1. *If h is subquadratic and $u \in S[0;2d]$ we have $v_0 \in S[2;2d]$, $v_1 \in S[1;2d]$, $v_n \in S[0;2d]$ and $v_N^\varepsilon \in S[0;5d]$ for all $n, N \geq 2$.*

2. *If h is polynomial in ξ, there are $w_N^\varepsilon \in S[(m_u, m_h + m_u);(2d,d)]$ such that*

$$\mathcal{R}^\varepsilon(\kappa;v_N^\varepsilon;\Theta^x,\Theta^y) = \mathcal{I}^\varepsilon(\kappa;w_N^\varepsilon;\Theta^x,\Theta^y)\,.$$

The first assertion of the corollary shows that in the case of our application all symbols v_n with $n \geq 2$ give rise to bounded operators. As mentioned before, this situation is different when general $\Theta^x, \Theta^y \in \mathcal{C}$ are considered. In this case, a complete expansion in the form of Proposition 7.3 would give rise to symbols v_n which grow quadratically for all $n \in \mathbb{N}$. For this reason, the composition result for the general case is restricted subquadratic Hamiltonians and restrain from the development of a hierarchy for the unbounded parts of the symbol.

7.5 Proposition (Composition with PDOs)**.** *Let $h \in S[2;2d]$ be a subquadratic symbol, κ a canonical transformation of class $\mathcal{B}$, $u \in S[0;2d]$ and $\Theta^x, \Theta^y \in \mathcal{C}$. There are $v_0 \in S[3;2d]$ and $v_n \in S[0;2d]$ $n \geq 1$ such that for any $N \in \mathbb{N}$ there is $v_{N+1}^\varepsilon \in S[2N+1;5d]$ with*

$$\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y) = \mathcal{I}^\varepsilon\left(\kappa;\sum_{n=0}^{N}\varepsilon^n v_n;\Theta^x,\Theta^y\right) + \mathcal{R}^\varepsilon\left(\kappa;v_{N+1}^\varepsilon;\Theta^x,\Theta^y\right)$$

as operators on $\mathcal{S}(\mathbb{R}^d)$, where v_{N+1}^ε is such that

$$\left\|\mathcal{R}^\varepsilon\left(\kappa;v_{N+1}^\varepsilon;\Theta^x,\Theta^y\right)\right\|_{L^2\to L^2} \leq C\varepsilon^{N+1}.$$

The explicit expressions for v_0 *and* v_1 *are*

$$v_0(q,p,x) = u(q,p)(h\circ\kappa)(q,p) + u(q,p)\left((h_x + i\Theta^x h_\xi)\circ\kappa\right)^\dagger(q,p)(x - X^\kappa(q,p)) \tag{7.7}$$

and

$$v_1(q,p) = u(q,p)\frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\left[\partial_z(h_x\circ\kappa(q,p)) + i\Theta^x\partial_z(h_\xi\circ\kappa(q,p))\right]\right), \tag{7.8}$$

whereas the symbols v_n *with* $n \geq 2$ *are given as*

$$v_n = L'_n[h;\kappa;\Theta^x,\Theta^y]u,$$

where the $L'_n[h;\kappa;\Theta^x,\Theta^y]$ *are linear differential operators in* (q,p) *of degree* n *whose coefficients are rational functions of* $\partial^\alpha_{(x,\xi)}h, 2 \leq |\alpha| \leq 2n$ *and* $\partial^\alpha_{(q,p)}F^\kappa, |\alpha| \leq n$.

At first sight is seems strange that the symbol $v^\varepsilon_{N+1} \in S[2N+1;5d]$ should give rise to a bounded operator. This is explained by the fact that the growth of the symbol comes only from terms of the form $u^\varepsilon(x,\xi,x',q,p)(x - X^\kappa(q,p))^\alpha(y-q)^\beta$ with $u^\varepsilon \in S[0;5d]$.

The situation of time-derivatives of FIOs is comparable to that of the composition with PDOs: Whereas we can give a full asymptotic expansion of the symbol in the case $\Theta^x,\Theta^y \in \mathcal{C}_{\mathrm{const}}$, the general case yields a more complicated result. We have

7.6 Proposition. *Let* $u \in C(\mathbb{R}, S[m;2d])$ *be a family of time-dependent symbols with* $u(\cdot,q,p) \in C^1(\mathbb{R},\mathbb{C})$ *and* $(\frac{d}{dt}u)(t,\cdot,\cdot) \in S[m;2d]$, κ^t *a* C^1*-family of canonical transformations of class* $\mathcal{B}$, $\Theta^x \in C^1(\mathbb{R},\mathcal{C}_{\mathrm{const}})$ *and* $\Theta^y \in \mathcal{C}_{\mathrm{const}}$. *We have*

$$i\varepsilon\frac{d}{dt}\mathcal{I}^\varepsilon\left(\kappa^t;u;\Theta^x(t),\Theta^y\right) = \mathcal{I}^\varepsilon\left(\kappa^t;\sum_{n=0}^{2}\varepsilon^n v_n;\Theta^x(t),\Theta^y\right)$$

with

$$v_0(t,q,p) = u(t,q,p)\left(-\frac{d}{dt}S^{\kappa^t}(q,p) + \frac{d}{dt}X^{\kappa^t}(q,p)\cdot\Xi^{\kappa^t}(q,p)\right) \tag{7.9}$$

$$\begin{aligned} v_1(t,q,p) = {} & i\frac{d}{dt}u(t,q,p) \\ & + \mathrm{div}_z\left(\left(\frac{d}{dt}\Xi^{\kappa^t}(q,p) - i\Theta^x(t)\frac{d}{dt}X^{\kappa^t}(q,p)\right)^\dagger \mathcal{Z}^{-1}(t,q,p)u(t,q,p)\right) \\ & - \frac{i}{2}u(t,q,p)\mathrm{tr}\left(\mathcal{Z}^{-1}(t,q,p)X_z^{\kappa^t}(q,p)\frac{d}{dt}\Theta^x(t)\right), \end{aligned} \tag{7.10}$$

and

$$v_2(t,q,p) = -\sum_{k=1}^{d}\mathrm{div}_z\left(\partial_{z_k}\left(\frac{d}{dt}\Theta^x(t)\mathcal{Z}^{-1}(t,q,p)e_k\,u(q,p)\right)^\dagger \mathcal{Z}^{-1}(t,q,p)\right), \tag{7.11}$$

where $v_0,v_1,v_2 \in C\left(\mathbb{R},S[m;2d]\right)$.

For the general case, we have

7.7 Proposition. *Let* $u \in C(\mathbb{R},S[0;2d])$ *be a family of time-dependent symbols with* $u(\cdot,q,p) \in C^1(\mathbb{R},\mathbb{C})$ *and* $(\frac{d}{dt}u)(t,\cdot,\cdot) \in S[0;2d]$, κ^t *a* C^1 *family of canonical transformations of class* $\mathcal{B}$,

$\Theta^x \in C^1(\mathbb{R}, \mathcal{C})$ and $\Theta^y \in \mathcal{C}$. There are $v_0 \in S[2; 2d]$ and $v_n \in S[0; 2d]$ $n \geq 1$ such that for any $N \in \mathbb{N}$ there is $v^\varepsilon_{N+1} \in S[2N+1; 5d]$ with

$$\frac{d}{dt}\mathcal{I}^\varepsilon(\kappa; u; \Theta^x(t), \Theta^y) = \mathcal{I}^\varepsilon\left(\kappa; \sum_{n=0}^{N} \varepsilon^n v_n; \Theta^x(t), \Theta^y\right) + \mathcal{I}^\varepsilon\left(\kappa; v^\varepsilon_{N+1}; \Theta^x(t), \Theta^y\right),$$

where v^ε_{N+1} is such that

$$\left\|\mathcal{I}^\varepsilon\left(\kappa^t; v^\varepsilon_{N+1}; \Theta^x(t), \Theta^y\right)\right\|_{L^2 \to L^2} = O(\varepsilon^{N+1}).$$

The explicit expressions for v_0 and v_1 are

$$\begin{aligned} v_0(t,q,p) &= u(t,q,p)\left(-\frac{d}{dt}S^{\kappa^t} + \frac{d}{dt}X^{\kappa^t} \cdot \Xi^{\kappa^t}\right) \\ &\quad - u(t,q,p)\left(\frac{d}{dt}\Xi^{\kappa^t} - i\Theta^x(t)\frac{d}{dt}X^{\kappa^t}\right)^\dagger (x - X^\kappa(q,p)) \end{aligned} \tag{7.12}$$

$$v_1(t,q,p) = i\frac{d}{dt}u(t,q,p) - \frac{i}{2}u(t,q,p)\operatorname{tr}\left(\mathcal{Z}^{-1}(t,q,p)X_z^{\kappa^t}(q,p)\frac{d}{dt}\Theta^x(t)\right), \tag{7.13}$$

whereas the symbols v_n with $n \geq 2$ are given as

$$v_n = L_n[\kappa^t; \Theta^x, \Theta^y]u,$$

where the $L_n[\kappa^t; \Theta^x, \Theta^y]$ are linear differential operators in (q,p) of degree n whose coefficients are rational functions of $\partial^\alpha_{(q,p)}F^\kappa, |\alpha| \leq n$.

To simplify the discussion of the Ehrenfest-timescale, we collect the assumptions we make for this case in the following shorthand description.

Ehrenfest case As the Ehrenfest case we understand the situation, where

1. $T = T(\varepsilon) = C_T\,|\log(\varepsilon)|$ for some $C_T > 0$.
2. $\kappa = \kappa^{(t,s)}$ arises from a classical Hamiltonian h which fulfills the assumptions of Proposition 2.7.
3. There are $\varepsilon_0 > 0, \rho_0 > 0$ such that the symbol $u^\varepsilon \in S[0; 4d]$ allows for a bound of the form
$$\left\|\partial^\alpha_{(x,y,q,p)}u^\varepsilon\right\|_{L^\infty(\mathbb{R}^{4d})} \leq C_\rho \varepsilon^{-\rho}$$
for all $\varepsilon \leq \varepsilon_0$ and $\rho \leq \rho_0$.
4. The matrices Θ^x and Θ^y allow for lower bounds of the form
$$\Theta^x, \Theta^y \geq C_\rho \varepsilon^\rho$$
for all $\varepsilon \leq \varepsilon_0$ and $\rho \leq \rho_0$.

The form of the symbol yields the following corollary.

7.8 Corollary. *Consider the Ehrenfest case.*

1. *For the symbols of Proposition 7.3 we have*

$$\left\|\partial^\alpha_{(q,p)} v_k\right\|_{L^\infty} \le C_\rho \varepsilon^{-\rho} \quad \forall n \ge 2 \quad \textit{and} \quad \left\|\partial^\alpha_{(x,\xi,x',y,q,p)} v^\varepsilon_N\right\|_{L^\infty} \le C_\rho \varepsilon^{-\rho}.$$

2. *In the situation of Proposition 7.5, we have the bounds*

$$\left\|\partial^\alpha_{(q,p)} v_k\right\|_{L^\infty} \le C_\rho \varepsilon^{-\rho} \quad \forall n \ge 1$$

and

$$\left\|\mathcal{R}^\varepsilon\big(\kappa; v^\varepsilon_{N+1}; \Theta^x, \Theta^y\big)\right\|_{L^2 \to L^2} \le C_\rho \varepsilon^{N+1-\rho}.$$

3. *For the symbols of Proposition 7.6 we have*

$$\left\|\partial^\alpha_{(q,p)} v_2\right\|_{L^\infty} \le C_\rho \varepsilon^{-\rho}.$$

4. *In the situation of Proposition 7.7, we have the bounds*

$$\left\|\partial^\alpha_{(q,p)} v_k\right\|_{L^\infty} \le C_\rho \varepsilon^{-\rho} \quad \forall n \ge 1$$

and

$$\left\|\mathcal{I}^\varepsilon\big(\kappa; v^\varepsilon_{N+1}; \Theta^x, \Theta^y\big)\right\|_{L^2 \to L^2} \le C_\rho \varepsilon^{N+1-\rho}.$$

In all cases, ρ can be made arbitrary small if C_T chosen small enough.

7.2 Proofs

The proof of the composition results strongly rely on integration by parts which convert deviations from the classical flow into an ε-hierarchy from the symbol. To keep the results free from too many technical details, we develop this machinery before we come to the core of the proofs. To simplify the notation, we introduce the following relation on the symbol spaces.

7.9 Definition (Equivalent symbols)**.**
Two symbols $u, v \in S[+\infty; 4d]$ and $u', v' \in S[+\infty; 6d]$ respectively are called ***equivalent with respect to*** *κ, if*

$$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) = \mathcal{I}^\varepsilon(\kappa; v; \Theta^x, \Theta^y) \quad \textit{and} \quad \mathcal{R}^\varepsilon\big(\kappa; u'; \Theta^x, \Theta^y\big) = \mathcal{R}^\varepsilon\big(\kappa; v'; \Theta^x, \Theta^y\big) \quad \textit{resp.},$$

where the identity holds as operators from $\mathcal{S}(\mathbb{R}^d)$ into $\mathcal{S}(\mathbb{R}^d)$. In both cases, we write $u \sim v$.

7.2.1 A hierarchy for a certain class of symbols

The fundamental observation to establish a ε-hierarchy is already contained in Corollary 4.12. There it is shown that deviations from the positions q and $X^\kappa(q,p)$ are related to the asymptotic behavior in ε. In the following section we will present more precise results on this behavior via integration by parts in the variables q and p. The results in this section are stated for the operators $\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)$, but of course anaogous results also hold for $\mathcal{R}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)$, when the symbol classes are adopted accordingly.

The central observation to establish the hierarchy is the equation

$$\begin{pmatrix}\Phi^\kappa_q\\ \Phi^\kappa_p\end{pmatrix} = W(q,p)\begin{pmatrix}x-X^\kappa(q,p)\\ y-q\end{pmatrix} + \frac{i}{2}\begin{pmatrix}\Theta^x_q(q,p)(x-X^\kappa(q,p))^2+\Theta^y_q(q,p)(y-q)^2\\ \Theta^x_p(q,p)(x-X^\kappa(q,p))^2+\Theta^y_p(q,p)(y-q)^2\end{pmatrix}, \tag{7.14}$$

with

$$W(q,p) := \left(\begin{array}{c|c} (F^\kappa)^\dagger(q,p)\begin{pmatrix}-i\Theta^x(q,p)\\ \mathrm{id}\end{pmatrix} & \begin{matrix}-i\Theta^y(q,p)\\ -\mathrm{id}\end{matrix}\end{array}\right)$$

where we abused notation by writing

$$\Theta_q x^2 := \left([\partial_{q_1}\Theta]\,x^2 \quad [\partial_{q_2}\Theta]\,x^2 \quad \dots \quad [\partial_{q_d}\Theta]\,x^2\right)^\dagger.$$

The matrix $W(q,p) = W^\kappa[\Theta^x,\Theta^y](q,p)$ is "well-behaved":

7.10 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$ and $\Theta^x,\Theta^y\in\mathcal{C}$. The matrix $W^\kappa[\Theta^x,\Theta^y]$ is invertible with $(W^\kappa[\Theta^x,\Theta^y])^{-1}(q,p)\in S[0;2d]$. In the Ehrenfest case, we have*

$$\left\|\partial^\alpha_{(q,p)}W^\kappa[\Theta^x,\Theta^y]\right\|_{L^\infty_{(q,p)}} \le C_\rho\varepsilon^{-\rho} \quad \text{and} \quad \left\|\partial^\alpha_{(q,p)}\left(W^\kappa[\Theta^x,\Theta^y]\right)^{-1}\right\|_{L^\infty_{(q,p)}} \le C_\rho\varepsilon^{-\rho}$$

for all $\alpha\in\mathbb{N}^d$, where ρ can be made arbitrary small if C_T chosen small enough.

The proof of the statement is found in the appendix. We exploit equation (7.14) by integration by parts with respect to q and p:

7.11 Lemma. *Let $u\in S[m;4d]$ and $V\in C^\infty(\mathbb{R}^{2d},\mathbb{C})$. Then*

$$V\cdot\begin{pmatrix}x-X^\kappa\\ y-q\end{pmatrix}u \sim \varepsilon v + w$$

where $v\in S[m;4d]$ and $w\in S[m+2;4d]$ are given by

$$v(x,y,q,p) = i\operatorname{div}_{(q,p)}\left(V^\dagger W^{-1}(q,p)u(x,y,q,p)\right)$$

and

$$w(x,y,q,p) = -\frac{i}{2}V\cdot W^{-1}(q,p)\begin{pmatrix}\Theta^x_q(x-X^\kappa)^2+\Theta^y_q(y-q)^2\\ \Theta^x_p(x-X^\kappa)^2+\Theta^y_p(y-q)^2\end{pmatrix}u(x,y,q,p)$$

In particular $w=0$ if $\Theta^x,\Theta^y\in\mathcal{C}_{\mathrm{const}}$.

As we assume that the reader is familiar with the oscillatory integral machinery after the study of Part II we do not give a detailed technical proof here. Furthermore, we notice that this Lemma contains all relevant information to establish Corollary 7.8.

The additional growth in w comes only from terms of the form $u(y-q,x-X^\kappa(q,p))^\alpha$, which do not influence the boundedness of the operator $\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)$, so iterative applications of Lemma 7.11 yield

7.12 Proposition. *Let $u \in S[0;2d]$ and $|\gamma| \geq 1$. There are $v_n \in S[0;2d], n \in \mathbb{N}$ such that for all $N \in \mathbb{N}$ there is $v^\varepsilon_{N+1} \in S[2N+1;4d]$ such that*

$$u(q,p)(x - X^\kappa, y-q)^\gamma \sim \sum_{k=\left\lceil \frac{|\gamma|}{2} \right\rceil}^{N} \varepsilon^k v_k(q,p) + v^\varepsilon_{N+1}, \tag{7.15}$$

where v^ε_{N+1} is of the form

$$v^\varepsilon_{N+1} = \sum_{k+\frac{|\alpha|}{2} \geq N+1} \varepsilon^k v_{k,\alpha,N}(q,p)(y-q, x - X^\kappa(q,p))^\alpha$$

with $v_{k,\alpha,N} \in S[0;2d]$. In particular

$$\left\| \mathcal{I}^\varepsilon\left(\kappa; v^\varepsilon_{N+1}; \Theta^x, \Theta^y\right) \right\|_{L^2 \to L^2} \leq C\varepsilon^{N+1}$$

and

$$\|\mathcal{I}^\varepsilon(\kappa; u(x - X^\kappa, y-q)^\gamma; \Theta^x, \Theta^y)\|_{L^2 \to L^2} \leq C\varepsilon^{\lceil |\gamma|/2 \rceil}.$$

In the Ehrenfest-case, we have $C = C(\varepsilon) \leq C(\rho)\varepsilon^{-\rho}$.

Proof. For $N = 0$ the result follows directly from Lemma 7.11 and Corollary 4.12. Assume that the existence of the v_n and an expansion of the form (7.15) is shown for $n \leq N$ with $N \in \mathbb{N}$. We construct v_{n+1} and v^ε_{N+1} in the following way: We set

$$w(x,y,q,p) := \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} \varepsilon^k v_{k,\alpha,N}(q,p)(y-q, x - X^\kappa(q,p))^\alpha.$$

By Corollary 4.12 every term in this sum is of order $O(\varepsilon^{k+\frac{|\alpha|}{2}}) = O(\varepsilon^{n+1})$ or higher in the sense that the operator with this symbol has L^2-operator norm of this order. Our aim is to translate this ε-dependency into a symbol of the form $\varepsilon^{n+1} v_{n+1}$.

Assuming for simplicity that $\alpha_1 \neq 0$ for all terms in the sum, an application of Lemma 7.11 yields

$$\begin{aligned} w \sim -\frac{i}{2} \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} & \varepsilon^k e_1^\dagger W^{-1}(q,p) \begin{pmatrix} \Theta^x_q (x - X^\kappa)^2 + \Theta^y_q (y-q)^2 \\ \Theta^x_p (x - X^\kappa)^2 + \Theta^y_p (y-q)^2 \end{pmatrix} \\ & \times v_{k,\alpha,N}(q,p)(y-q, x-X^\kappa(q,p))^{\alpha - e_1} \\ + \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} & i\varepsilon^{k+1} \operatorname{div}_{(q,p)} \left(e_1^\dagger W^{-1}(q,p) v_{k,\alpha,N}(q,p)(y-q, x-X^\kappa(q,p))^{\alpha - e_1} \right). \end{aligned}$$

The product rule splits the last term of the expression into a polynomial of degree $|\alpha| - 1$ and one of degree $|\alpha| - 2$:

$$w \sim -\frac{i}{2} \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} \varepsilon^k e_1^\dagger W^{-1}(q,p) \begin{pmatrix} \Theta_q^x(x - X^\kappa)^2 + \Theta_q^y(y-q)^2 \\ \Theta_p^x(x - X^\kappa)^2 + \Theta_p^y(y-q)^2 \end{pmatrix} \tag{7.16}$$

$$\times v_{k,\alpha,N}(q,p)(y-q, x - X^\kappa(q,p))^{\alpha - e_1}$$

$$+ \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} i\varepsilon^{k+1} \mathrm{div}_{(q,p)} \left(e_1^\dagger W^{-1}(q,p) v_{k,\alpha,N}(q,p) \right) (y-q, x - X^\kappa(q,p))^{\alpha - e_1} \tag{7.17}$$

$$- \sum_{k+\frac{|\alpha|}{2} \in \{n+1, n+\frac{3}{2}\}} i\varepsilon^{k+1} e_1^\dagger W^{-1}(q,p) v_{k,\alpha,N}(q,p) \tag{7.18}$$

$$\times \sum_{l=1}^{2d} (\alpha - e_1)_l \, (y-q, x - X^\kappa(q,p))^{\alpha - e_1 - e_l} \partial_{z_l}(q, X^\kappa(q,p))^{e_l}$$

The essential observation from this computation is the following: Due to Corollary 4.12, (7.16) and (7.17) are of order $k + \frac{|\alpha|}{2} + \frac{1}{2}$ in ε. Thus those terms have been pushed by half an order in ε and may be put into the remainder after a possible repetition of the procedure. On the other hand, (7.18) is still of order $k + \frac{|\alpha|}{2}$ but with its degree in $(x - X^\kappa(q,p), y - q)$ lowered by two. Thus one can iterate the procedure unital all $(x - X^\kappa(q,p), y-q)$-dependence is removed and the result follows. □

An important special case occurs for monomials in $(x - X^\kappa(q,p))$.

7.13 Corollary. *Let $u \in S[m; 4d]$ and $V \in \mathbb{C}(\mathbb{R}^{2d})$. Then*

$$V \cdot (x - X^\kappa)\, u \sim \varepsilon(v + v') + w$$

where $v, v' \in S[m; 4d]$ and $w \in S[m+2; 4d]$ are given by

$$v(x,y,q,p) = -\mathrm{div}_z \left(V^\dagger \mathcal{Z}^{-1}(q,p) u(x,y,q,p) \right)$$

$$v'(x,y,q,p) = -\sum_{k=1}^{d} u(x,y,q,p) V^\dagger \mathcal{Z}^{-1}(q,p) \left[\partial_{q_k} (\Theta^y)^{-1} \right] e_k$$

$$w(x,y,q,p) = \frac{1}{2} V \cdot \mathcal{Z}^{-1}(q,p) \left(\Theta_z^x(x - X^\kappa)^2 + \Theta_z^y(y-q)^2 \right) u(x,y,q,p).$$

In particular, $v' = w = 0$ if $\Theta^x, \Theta^y \in \mathcal{C}_{\mathrm{const}}$.

The result follows from the relation

$$i\partial_z \Phi^\kappa(q,p) = \mathcal{Z}(q,p)(x - X^\kappa(q,p))$$

by integration by parts in q and p.

To establish an asymptotic solution, we need precise information about the symbols, which arise in the compositions. Motivated by the form of the image of the FBI-transform and the close relation of our FIOs to the Anti-Wick-quantisation, we turn to the following creation and annihilation framework on the classical phase space. We introduce the "variables"

$$a\left(\frac{x+x'}{2}, \xi, q, p\right) := (\Theta^x(q,p))^{\frac{1}{2}} \frac{x+x'}{2} + i\,(\Theta^x(q,p))^{-\frac{1}{2}} \xi,$$

$$\overline{a}\left(\frac{x+x'}{2}, \xi, q, p\right) := (\Theta^x(q,p))^{\frac{1}{2}} \frac{x+x'}{2} - i\,(\Theta^x(q,p))^{-\frac{1}{2}} \xi$$

and their "dual operators"

$$\partial_a := -\frac{i}{2}\left(\Theta^x(q,p)\right)^{\frac{1}{2}}\partial_\xi + \left(\Theta^x(q,p)\right)^{-\frac{1}{2}}\partial_{x'}$$
$$\partial_{\overline{a}} := \frac{i}{2}\left(\Theta^x(q,p)\right)^{\frac{1}{2}}\partial_\xi + \left(\Theta^x(q,p)\right)^{-\frac{1}{2}}\partial_{x'},$$

which fulfill

$$\begin{pmatrix}\partial_a \\ \partial_{\overline{a}}\end{pmatrix}\begin{pmatrix}a & \overline{a}\end{pmatrix} = \begin{pmatrix}\mathrm{id} & 0 \\ 0 & \mathrm{id}\end{pmatrix}. \tag{7.19}$$

For a canonical transformation, we introduce a similar structure:

$$Z^\kappa(q,p) := \left(\Theta^x(q,p)\right)^{\frac{1}{2}} X^\kappa(q,p) + i\left(\Theta^x(q,p)\right)^{-\frac{1}{2}}\Xi^\kappa(q,p) \tag{7.20}$$
$$\overline{Z}^\kappa(q,p) := \left(\Theta^x(q,p)\right)^{\frac{1}{2}} X^\kappa(q,p) - i\left(\Theta^x(q,p)\right)^{-\frac{1}{2}}\Xi^\kappa(q,p).$$

We want to point out that $\overline{Z}^\kappa(q,p)$ is not the complex conjugate of $Z^\kappa(q,p)$ as $\Theta^x(q,p)$ is in general non-real.

The importance of these operators stems from the relations

$$\partial_a\Psi^\kappa = -i\left[\overline{a}\left(\frac{x+x'}{2},\xi\right) - \overline{Z}^\kappa\right] + 2i\left(\Theta^x\right)^{\frac{1}{2}}\left[x' - X^\kappa\right] \tag{7.21}$$

and

$$\partial_{\overline{a}}\Psi^\kappa = i\left[a\left(\frac{x+x'}{2},\xi\right) - Z^\kappa\right],$$

which allow to transform deviations of $Z^\kappa(q,p)$ and $\overline{Z}^\kappa(q,p)$ from a and $\overline{a}$.

7.14 Lemma. *Let $u \in S[+\infty; 6d]$. We have*

$$\left(a - Z^\kappa\right)_j u \sim \varepsilon\partial_{\overline{a}_j} u \tag{7.22}$$

and

$$\left(\overline{a} - \overline{Z}^\kappa\right)_j u \sim \varepsilon\partial_{a_j} u + 2u\left[\left(\Theta^x\right)^{\frac{1}{2}}\left(x' - X^\kappa(q,p)\right)\right]_j \tag{7.23}$$

7.2.2 Proofs of Propositions 7.3–7.7

With these preparations, we ready to prove the central composition results and start for the composition result for the case of constant and real matrices Θ^x and Θ^y.

Proof of Proposition 7.3. Let $\varphi \in \mathcal{S}(\mathbb{R}^d,\mathbb{C})$. The composition of $\mathrm{op}^\varepsilon(h)$ with the FIO applied to φ is given by

$$\begin{aligned}&\left[\mathrm{op}^\varepsilon(h)\mathcal{I}^\varepsilon(\kappa;u;\Theta^x,\Theta^y)\,\varphi\right](x)\\ &= \frac{1}{(2\pi\varepsilon)^{5d/2}}\int_{\mathbb{R}^{5d}} h\left(\frac{x+x'}{2},\xi\right) e^{\frac{i}{\varepsilon}\Psi^\kappa(x,\xi,x',y,q,p;\Theta^x,\Theta^y)} u(q,p)\varphi(y)\;dq\,dp\,dy\,dx'\,d\xi.\end{aligned}$$

We perform a Taylor-expansion of the symbol h in the complex variables a and $\overline{a}$ to order $2N$ around κ, compare Lemma 10.10. We get

$$\begin{aligned} h(x,\xi) = &\sum_{|\alpha+\beta|\le 2N} \frac{1}{\alpha!\beta!}\left(\left(\partial_a^\alpha \partial_{\overline{a}}^\beta h\right)\circ\kappa\right)(a-Z^\kappa)^\alpha \left(\overline{a}-\overline{Z}^\kappa\right)^\beta \\ &+ \sum_{|\alpha+\beta|=2N+1} (a-Z^\kappa)^\alpha \left(\overline{a}-\overline{Z}^\kappa\right)^\beta R_{\alpha,\beta}(a,\overline{a},q,p) \\ =:& \, h_{\mathrm{T}}\left(a-Z^\kappa, \overline{a}-\overline{Z}^\kappa\right) + h_{\mathrm{R}}(a,\overline{a},q,p), \end{aligned}$$

where

$$R_{\alpha,\beta}(x,\xi,q,p) = \frac{|\alpha+\beta|}{\alpha!\beta!}\int_0^1 \tau^{|\alpha+\beta|-1}\left(\partial_a^\alpha \partial_{\overline{a}}^\beta h\right)(x+\tau(X^\kappa - x), \xi + \tau(\Xi^\kappa - \xi))d\tau \in S[m_h;4d].$$

Using (7.22) and (7.19), we have

$$h_{\mathrm{T}}\left(a-Z^\kappa, \overline{a}-\overline{Z}^\kappa\right)u \sim \sum_{|\alpha+\beta|\le 2N} \frac{\varepsilon^{|\alpha|}}{\alpha!(\beta-\alpha)!}\left(\overline{a}-\overline{Z}^\kappa\right)^{\beta-\alpha}\left(\left(\partial_a^\alpha \partial_{\overline{a}}^\beta h\right)\circ\kappa\right)u. \tag{7.24}$$

As $\Theta^x, \Theta^y \in \mathcal{C}_{\mathrm{const}}$ Lemma 7.11 shows that $(x'-X^\kappa)u \sim \mathrm{div}_z\left(\mathcal{Z}^{-1}(q,p)u\right)$ and hence (7.23) yields

$$\left(\overline{a}-\overline{Z}^\kappa(q,p)\right)^\gamma v(q,p) \sim -2\varepsilon\mathrm{div}_z\left(e_1^\dagger (\Theta^x)^{\frac12}\mathcal{Z}^{-1}(q,p)\left(\overline{a}-\overline{Z}^\kappa(q,p)\right)^{\gamma-e_k} v(q,p)\right) \tag{7.25}$$

for any $\gamma \in \mathbb{N}^d$ with $\gamma_1 > 0$.

To iterate this procedure, we denote by $\#\gamma$ the number of non-zero elements of γ and rewrite (7.25) as

$$\begin{aligned} &\left(\overline{a}-\overline{Z}^\kappa(q,p)\right)^\gamma v(q,p) \\ \sim& -\frac{2\varepsilon}{\#\gamma}\sum_{k|\gamma_k\ne 0}\mathrm{div}_z\left(e_k^\dagger (\Theta^x)^{\frac12}\mathcal{Z}^{-1}(q,p)\left(\overline{a}-\overline{Z}^\kappa(q,p)\right)^{\gamma-e_k} v(q,p)\right) \\ =& \frac{\varepsilon}{\#\gamma}\sum_{k|\gamma_k\ne 0}\left[\sum_{m=1}^d (\gamma-e_k)_m\left(\overline{a}-\overline{Z}^\kappa\right)^{\gamma-e_k-e_m}(\mathcal{L}_{(e_k,e_m)}v) + \left(\overline{a}-\overline{Z}^\kappa\right)^{\gamma-e_k}(\mathcal{L}_{e_k}v)\right] \end{aligned} \tag{7.26}$$

where the linear differential operators $\mathcal{L}_{(e_k,e_m)}$ and $\mathcal{L}_{(e_k)}$ are given by

$$\begin{aligned} (\mathcal{L}_{(e_k,e_m)}v)(q,p) &:= 2e_k^\dagger (\Theta^x)^{\frac12}\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa e_m v(q,p) \\ (\mathcal{L}_{(e_k)}v)(q,p) &:= -2\mathrm{div}_z\left(e_k^\dagger (\Theta^x)^{\frac12}\mathcal{Z}^{-1}(q,p)v(q,p)\right). \end{aligned}$$

With the three sets

$$\Gamma_1 := \left\{\gamma \in \mathbb{N}^d \,\middle|\, |\gamma| = 1\right\}, \quad \Gamma_2 := \Gamma_1 \times \Gamma_1, \quad \Gamma := \Gamma_1 \cup \Gamma_2,$$

we have the following interpretation: the sum in (7.26) is taken over all possible reductions of the multi-index γ by elements of the "brick-sets" Γ_1 and Γ_2. After another integration by

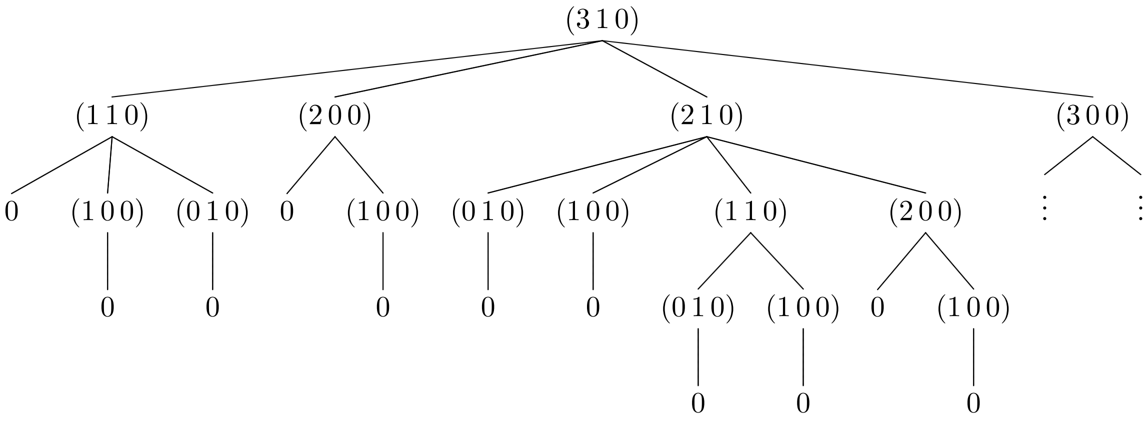

Figure 7.1: Decomposition of $\alpha = (3\,1\,0)$ with elements of Γ the length of each path of the tree corresponds to the order in ε to which it is contributing.

parts in all terms with $\left(\overline{a} - \overline{Z}^{\kappa}\right)$-dependence, the sum is taken over all possible reductions of γ by elements in $\Gamma \times \Gamma$, which may be considered as a two-step path in Γ, plus the terms which already led to $\gamma = 0$ in the first step. So after the removal of all $\left(\overline{a} - \overline{Z}^{\kappa}\right)$-dependence, the sum is taken over all possible paths in the "brick-set" Γ which reduce γ to zero, compare Figure 7.1.

To formalise this idea, we define the map

$$\begin{aligned} [\,\cdot\,] \quad &: \quad \Gamma \to \mathbb{N}^d \\ [\gamma] \quad &:= \quad \begin{cases} \gamma & \gamma \in \Gamma_1 \\ \gamma_1 + \gamma_2 & \gamma = (\gamma_1, \gamma_2) \in \Gamma_2 . \end{cases} \end{aligned}$$

Setting

$$\lambda(\gamma, \gamma_1, \ldots, \gamma_n) = \begin{cases} \left(\#(\gamma - \sum\limits_{l<n} [\gamma_l]) \right)^{-1} & \gamma_n \in \Gamma_1 \\ \left(\#(\gamma - \sum\limits_{l<n} [\gamma_l]) \right)^{-1} \left(\gamma - \sum\limits_{l<n} [\gamma_l] - e_j \right)_k & \gamma_n = (e_j, e_k) \in \Gamma_2, \end{cases}$$

we have

$$\left(\overline{a} - \overline{Z}^{\kappa}\right)^{\gamma} v \sim \sum_{\substack{\gamma_1 \ldots, \gamma_k \in \Gamma \\ [\gamma_1] + \ldots + [\gamma_k] = \gamma}} \varepsilon^k \lambda(\gamma, \gamma_1, \ldots, \gamma_k) \ldots \lambda(\gamma, \gamma_1, \gamma_2) \lambda(\gamma, \gamma_1) \left(\mathcal{L}_{\gamma_k} \ldots \mathcal{L}_{\gamma_1} v \right). \tag{7.27}$$

Combining this expression with (7.24), we obtain

$$h_{\mathrm{T}} u \sim \sum_{\substack{|\beta| \leq 2N \\ \alpha \leq \beta}} \sum_{\substack{\gamma_1 \ldots, \gamma_k \in \Gamma \\ [\gamma_1] + \ldots + [\gamma_k] = \beta - \alpha}} \frac{\varepsilon^{|\alpha| + k}}{\alpha! (\beta - \alpha)!} \left(\prod_{l=1}^{k} \lambda(\gamma, \gamma_1, \ldots, \gamma_l) \mathcal{L}_{\gamma_l} \right) \left(u \, \partial_a^{\alpha} \partial_{\overline{a}}^{\beta} h \circ \kappa \right).$$

Now k ranges between $\lceil|\beta-\alpha|/2\rceil$ and $|\beta-\alpha|$, so we have

$$\begin{aligned}&L_n[h;\kappa;\Theta^x,\Theta^y]u\\ &=\sum_{\substack{n\le|\alpha+\beta|\le 2n\\ \alpha\le\beta}}\frac{1}{\alpha!(\beta-\alpha)!}\sum_{\substack{\gamma_1,\dots,\gamma_{n-|\alpha|}\in\Gamma\\ \lceil\gamma_1\rceil+\dots+\lceil\gamma_{n-|\alpha|}\rceil=\beta-\alpha}}\left(\prod_{l=1}^{n-|\alpha|}\lambda(\gamma,\gamma_1,\dots,\gamma_l)\mathcal{L}_{\gamma_l}\right)\left(u\,\partial_a^\alpha\partial_{\overline{a}}^\beta h\circ\kappa\right)\end{aligned}$$

where we use the convention

$$\sum_{\gamma_1,\dots,\gamma_{n-|\alpha|}}\prod_{l=1}^{n-|\alpha|}\lambda(\gamma,\gamma_1,\dots,\gamma_l)\mathcal{L}_{\gamma_l}=\mathrm{id}$$

for $n-|\alpha|=0$. Note that after the reduction of all creation and annihilation terms, the symbol arising from h_T is independent of x and ξ, so that we can apply Lemma 5.2 to turn the operator $\mathcal{R}^\varepsilon(\kappa;h_T;\Theta^x,\Theta^y)$ into the form $\mathcal{I}^\varepsilon(\kappa;v;\Theta^x,\Theta^y)$.

We develop the explicit expressions for the lowest order terms. The zeroth order term

$$(h\circ\kappa)\,u$$

is provided by $\alpha=\beta=0$. For the first order term, there are three contributions.

1. The terms with $|\beta|=1,\alpha=\beta$, which result in

$$\varepsilon\sum_{k=1}^{d}\left(\left(\left(\partial_{a_k}\partial_{\overline{a}_k}h\right)\circ\kappa\right)(q,p)\right)u(q,p)=\varepsilon\mathrm{tr}\left(\left(\left(\partial_a\partial_{\overline{a}}h\right)\circ\kappa\right)(q,p)\right)u(q,p).$$

2. The terms $|\beta|=1,\alpha=0$, which give

$$\begin{aligned}\varepsilon\sum_{k=1}^{d}\mathcal{L}_{e_k}\left(u\partial_{\overline{a}_k}h\circ\kappa\right)(q,p)&=2\varepsilon\sum_{k=1}^{d}\mathrm{div}_z\left(e_k^\dagger\left(\Theta^x\right)^{\frac12}\mathcal{Z}^{-1}(q,p)\left(\partial_{\overline{a}_k}h\circ\kappa\right)(q,p)u(q,p)\right)\\ &=-\mathrm{div}_z\left(\left(\left(h_x+i\Theta^x h_\xi\right)\circ\kappa\right)^\dagger(q,p)\mathcal{Z}^{-1}(q,p)u\right).\end{aligned}$$

3. The first order contribution of terms $|\beta|=2,\alpha=0$, which is

$$\begin{aligned}&\sum_{k,l=1}^{d}\frac{\varepsilon}{2}u(q,p)\mathcal{L}_{e_k,e_l}(\partial_{\overline{a}_k}\partial_{\overline{a}_l}h\circ\kappa)(q,p)\\ &=\sum_{k,l=1}^{d}\varepsilon e_k^\dagger\left(\Theta^x\right)^{\frac12}\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa e_l(\partial_{\overline{a}_k}\partial_{\overline{a}_l}h\circ\kappa)(q,p)u(q,p)\\ &=\sum_{k=1}^{d}\varepsilon e_k^\dagger\left(\Theta^x\right)^{\frac12}\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa\left(\left(\mathrm{Hess}_{\overline{a}}h\right)\circ\kappa\right)(q,p)e_k u(q,p)\\ &=\varepsilon\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa\left(\left(\mathrm{Hess}_{\overline{a}}h\right)\circ\kappa\right)(q,p)\left(\Theta^x\right)^{\frac12}\right)u(q,p).\end{aligned}$$

Recalling that

$$\mathcal{Z}(q,p) = (i\,(\Theta^y)^{-1} \quad \mathrm{id})(F^\kappa(q,p))^\dagger(-i\Theta^x \quad \mathrm{id})^\dagger = \partial_z Z^\kappa(q,p)\,(\Theta^x)^{\frac{1}{2}}\,, \tag{7.28}$$

the traces may be combined by an application of the chain rule

$$\begin{aligned}
&\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa\left((\mathrm{Hess}_{\overline{a}}h)\circ\kappa\right)(\Theta^x)^{\frac{1}{2}}\right) + \mathrm{tr}\left(((\partial_a\partial_{\overline{a}}h)\circ\kappa)\right)\\
&= \mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa\left((\mathrm{Hess}_{\overline{a}}h)\circ\kappa\right)(\Theta^x)^{\frac{1}{2}}\right) + \mathrm{tr}\left((\Theta^x)^{-\frac{1}{2}}\left((\partial_a\partial_{\overline{a}}h)\circ\kappa\right)(\Theta^x)^{\frac{1}{2}}\right)\\
&= \mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^\kappa\left((\mathrm{Hess}_{\overline{a}}h)\circ\kappa\right)(\Theta^x)^{\frac{1}{2}}\right) + \mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z Z^\kappa\left((\partial_a\partial_{\overline{a}}h)\circ\kappa\right)(\Theta^x)^{\frac{1}{2}}\right)\\
&= \mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\left[(\Theta^x)^{\frac{1}{2}}\left((\partial_{\overline{a}}h)\circ\kappa\right)\right]\right)\\
&= \frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\left[(((\partial_x + i\Theta^x\partial_\xi)h)\circ\kappa)\right]\right).
\end{aligned}$$

We turn to the discussion of h_R. Using (7.22) iteratively, we have

$$\begin{aligned}
&\sum_{|\alpha+\beta|=2N+1}(a-Z^\kappa)^\alpha\left(\overline{a}-\overline{Z}^\kappa\right)^\beta R_{\alpha,\beta}\left(a,\overline{a},q,p\right)\\
&\sim \sum_{|\alpha+\beta|=2N+1}\varepsilon^{|\alpha|}\partial_{\overline{a}}^\alpha\left[\left(\overline{a}-\overline{Z}^\kappa\right)^\beta R_{\alpha,\beta}\left(a,\overline{a},q,p\right)\right]\\
&\sim \sum_{|\alpha+\beta|=2N+1}\sum_{\gamma\le\alpha}\varepsilon^{|\alpha|}\binom{\alpha}{\gamma}\frac{\beta!}{(\beta-\gamma)!}\left(\overline{a}-\overline{Z}^\kappa\right)^{\beta-\gamma}\left(\partial_{\overline{a}}^{\alpha-\gamma}R_{\alpha,\beta}\right)\left(a,\overline{a},q,p\right).
\end{aligned}$$

Now by integration by parts using (7.23), we see that the $\left(\overline{a}-\overline{Z}^\kappa\right)^{\beta-\gamma}$-term can be converted into a sum of symbols of orders $\lceil|\beta-\gamma|/2\rceil$ to $\lceil|\beta-\gamma|\rceil$ and therefore the remainder is of order

$$|\alpha| + \lceil|\beta-\gamma|/2\rceil \ge \lceil 2|\alpha| + |\beta-\gamma|\rceil/2 \ge \lceil 2N+1\rceil/2 = N+1$$

in the semiclassical parameter ε. □

Next, we show the composition result of PDOs and FIOs in the general case.

Proof of Proposition 7.5. The proof is in large parts identical to the one of Proposition 7.3. Exactly the same arguments as before yield (7.24), which reads

$$h_{\mathrm{T}}\left(a-Z^\kappa,\overline{a}-\overline{Z}^\kappa\right)u \sim \sum_{|\alpha+\beta|\le 2N}\frac{\varepsilon^{|\alpha|}}{\alpha!(\beta-\alpha)!}\left(\overline{a}-\overline{Z}^\kappa\right)^{\beta-\alpha}\left(\left(\partial_a^\alpha\partial_{\overline{a}}^\beta h\right)\circ\kappa\right)u.$$

The difference lies in the fact that the conversion of the creation terms $(\overline{a}-\overline{Z}^\kappa(q,p))$ is more complicated, as the full result of Lemma 7.11 has to be applied. Therefore, we will not reduce these terms in one step but convert them to $(x'-X^\kappa(q,p))$ factors first. An application of Proposition 7.12 will then complete the proof.

From (7.21) and (7.19) we deduce inductively that

$$\left(\overline{a}-\overline{Z}^\kappa\right)^\gamma e^{\frac{i}{\varepsilon}\Psi} = \left(\varepsilon\partial_a + 2\,(\Theta^x)^{\frac{1}{2}}\,(x'-X^\kappa)\right)^\gamma e^{\frac{i}{\varepsilon}\Psi} \tag{7.29}$$

and hence

$$
\begin{aligned}
&h_{\mathrm{T}}\left(a-Z^{\kappa},\overline{a}-\overline{Z}^{\kappa}\right)u\\
&\sim\sum_{|\alpha+\beta|\le 2N}\frac{\varepsilon^{|\alpha|}}{\alpha!(\beta-\alpha)!}\left(\left(\partial_a^{\alpha}\partial_{\overline{a}}^{\beta}h\right)\circ\kappa\right)\left(-\varepsilon\partial_a+2\left(\Theta^x\right)^{\frac12}\left(x'-X^{\kappa}\right)\right)^{\beta-\alpha}u\\
&=\sum_{|\alpha+\beta|\le 2N}\frac{\varepsilon^{|\alpha|}}{\alpha!(\beta-\alpha)!}\left(\left(\partial_a^{\alpha}\partial_{\overline{a}}^{\beta}h\right)\circ\kappa\right)\left(-\varepsilon\partial_{x'}+2(x'-X^{\kappa})\right)^{\beta-\alpha}u. \qquad (7.30)
\end{aligned}
$$

Note that u is independent of x', so that we have

$$\left(-\varepsilon\partial_{x'}+2(x'-X^{\kappa})\right)^{\beta-\alpha}u=\sum_{2k+|\gamma|=|\beta-\alpha|}a_{k,\gamma}\varepsilon^k(x'-X^{\kappa})^{\gamma}u$$

with ε-independent coefficients $a_k,\gamma\in\mathbb{C}$. Thus an application of Proposition 7.12 yields the existence of an expansion in the claimed form.

We turn to the explicit expressions of v_0 and v_1. As h is subquadratic, unbounded parts arise only from the Taylor-polynomial of order one. Using (7.30), we have

$$
\begin{aligned}
&h\left(Z^{\kappa}(q,p),\overline{Z}^{\kappa}(q,p)\right)+\sum_{j=1}^{d}\left(\partial_{\overline{a}_j}h\circ\kappa\right)(q,p)(\overline{a}-\overline{Z}^{\kappa}(q,p))_j u(q,p)\\
&\sim\left(h\circ\kappa\right)(q,p)+2e_j^{\dagger}\left(\partial_{\overline{a}_j}h\circ\kappa\right)(q,p)\left(\Theta^x(q,p)\right)^{\frac12}(x'-X^{\kappa})u(q,p)\\
&=\left(h\circ\kappa\right)(q,p)+\left(\left(\left(\partial_x+i\Theta^x\partial_{\xi}\right)h\right)\circ\kappa\right)(q,p)^{\dagger}(x'-X^{\kappa})u(q,p).
\end{aligned}
$$

The symbol v_1 arises from the second order derivatives of h. As the relation (7.28) is not valid for non-constant Θ^x and Θ^y we cannot use the chain rule to obtain the explicit expression, but we have

$$
\begin{aligned}
&(X_z\left(\Theta^x\right)^{\frac12}-i\Xi_z\left(\Theta^x\right)^{-\frac12})\partial_{\overline{a}}\partial_{\overline{a}}h\left(\Theta^x\right)^{\frac12}+\mathcal{Z}(q,p)\left(\Theta^x\right)^{-\frac12}\partial_a\partial_{\overline{a}}h\left(\Theta^x\right)^{\frac12}\\
&=(X_z\left(\Theta^x\right)^{\frac12}-i\Xi_z\left(\Theta^x\right)^{-\frac12})\partial_{\overline{a}}((\partial_x+i\Theta^x\partial_{\xi})\,h)+\mathcal{Z}(q,p)\left(\Theta^x\right)^{-\frac12}\partial_a((\partial_x+i\Theta^x\partial_{\xi})\,h)\\
&=(X_z\left(\Theta^x\right)^{\frac12}-i\Xi_z\left(\Theta^x\right)^{-\frac12})\partial_{\overline{a}}\left((\partial_x+i\Theta^x\partial_{\xi})\,h\right)+(X_z\left(\Theta^x\right)^{\frac12}+i\Xi_z\left(\Theta^x\right)^{-\frac12})\partial_a((\partial_x+i\Theta^x\partial_{\xi})\,h)\\
&=(X_z\partial_x+\Xi_z\partial_{\xi})((\partial_x+i\Theta^x\partial_{\xi})\,h)
\end{aligned}
$$

and thus

$$
\begin{aligned}
&\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\partial_z\overline{Z}^{\kappa}\left(\left(\mathrm{Hess}_{\overline{a}}h\right)\circ\kappa\right)\left(\Theta^x\right)^{\frac12}\right)+\mathrm{tr}\left(\left(\left(\partial_a\partial_{\overline{a}}h\right)\circ\kappa\right)\right)\\
&=\frac12\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\left[\partial_z(h_x\circ\kappa(q,p))+i\Theta^x\partial_z(h_{\xi}\circ\kappa(q,p))\right]\right).
\end{aligned}
$$

The treatment of the remainder is analogue to the proof of Proposition 7.3. Again using (7.22), we have

$$
\begin{aligned}
&\sum_{|\alpha+\beta|=2N+1}(a-Z^{\kappa})^{\alpha}\left(\overline{a}-\overline{Z}^{\kappa}\right)^{\beta}R_{\alpha,\beta}\left(a,\overline{a},q,p\right)\\
&\sim\sum_{|\alpha+\beta|=2N+1}\sum_{\gamma\le\alpha}\varepsilon^{|\alpha|}\binom{\alpha}{\gamma}\frac{\beta!}{(\beta-\gamma)!}\left(\overline{a}-\overline{Z}^{\kappa}\right)^{\beta-\gamma}\left(\partial_{\overline{a}}^{\alpha-\gamma}R_{\alpha,\beta}\right)(a,\overline{a},q,p)
\end{aligned}
$$

and a combination of (7.29) and Proposition 7.12 concludes the proof. □

Finally, we show the results on the time-derivative of FIOs

Proof of Proposition 7.6. By direct computation, the strong time-derivative of an FIO on $\mathcal{S}(\mathbb{R}^d)$ is given as

$$i\varepsilon \frac{d}{dt}\mathcal{I}^\varepsilon\left(\kappa^t; u; \Theta^x, \Theta^y\right) = \mathcal{I}^\varepsilon\left(\kappa^t; v; \Theta^x, \Theta^y\right)$$

where

$$\begin{aligned} &v(x,y,q,p) \\ &= -\frac{d}{dt}S^{\kappa^t}(q,p)u + \Xi^{\kappa^t}(q,p)\cdot\frac{d}{dt}X^{\kappa^t}(q,p)u - \left(\frac{d}{dt}\Xi^{\kappa^t} - i\Theta^x\frac{d}{dt}X^{\kappa^t}\right)(x - X^{\kappa^t})u \\ &\quad - i\left(\frac{d}{dt}\Theta^x\right)(x - X^\kappa(q,p))^2/2u + i\varepsilon\frac{d}{dt}u. \end{aligned} \tag{7.31}$$

By iterative applications of Corollary 7.13 we have

$$\begin{aligned} &v(x,y,q,p) \\ &\sim -\frac{d}{dt}S^{\kappa^t}(q,p)u + \Xi^{\kappa^t}(q,p)\cdot\frac{d}{dt}X^{\kappa^t}(q,p)u \\ &\quad + \varepsilon \mathrm{div}_z\left(\left(\frac{d}{dt}\Xi^{\kappa^t} - i\Theta^x\frac{d}{dt}X^{\kappa^t}\right)^\dagger \mathcal{Z}^{-1}(q,p)u\right) + i\varepsilon\frac{d}{dt}u \\ &\quad + \frac{i\varepsilon}{2}\mathrm{div}_z\left(\left[\left(\frac{d}{dt}\Theta^x\right)(x - X^\kappa(q,p))\right]^\dagger \mathcal{Z}^{-1}(q,p)u\right). \end{aligned}$$

Now the last term splits into terms of order ε and ε^2:

$$\begin{aligned} &\mathrm{div}_z\left(\left[\left(\frac{d}{dt}\Theta^x\right)(x - X^\kappa(q,p))\right]^\dagger \mathcal{Z}^{-1}(q,p)u\right) \\ &= \mathrm{tr}\left(\partial_z\left[\left(\frac{d}{dt}\Theta^x\right)(x - X^\kappa(q,p))\right]^\dagger \mathcal{Z}^{-1}(q,p)u\right) \\ &= -u\,\mathrm{tr}\left(\mathcal{Z}^{-1}(q,p)\left(X_z^\kappa(q,p)\frac{d}{dt}\Theta^x\right)u\right) \\ &\quad + 2\sum_{k=1}^d \mathrm{div}_z\left(\partial_{z_k}\left(\frac{d}{dt}\Theta^x(t)\mathcal{Z}^{-1}(t,q,p)e_k\,u(q,p)\right)^\dagger \mathcal{Z}^{-1}(t,q,p)\right), \end{aligned}$$

which yields the result. □

Proof of Proposition 7.7. The proof is analogous to the proof of Proposition 7.6. The difference lies in the treatment of the symbol (7.31), whose unbounded parts are not converted into orders in ε and in the use of Proposition 7.12 for the existence of a hierarchy. □

8 Uniform approximation of the propagator

In this section, we use the composition results and the results on time-derivatives to establish an approximation of the unitary group by Fourier Integral Operators.

8.1 Statement and proof of the main result

8.1 Theorem. *Let $U^\varepsilon(t,s)$ be the propagator associated to the time-dependent Schrödinger-equation*

$$i\varepsilon\frac{d}{dt}\psi^\varepsilon(t) = \mathrm{op}^\varepsilon(h^\varepsilon(t))\psi^\varepsilon(t), \qquad \psi^\varepsilon(s) = \psi^\varepsilon_s \in L^2(\mathbb{R}^d)$$

for $-T < s,t < T$, where $h^\varepsilon(t) = h_0(t) + \varepsilon h_1(t)$ with subquadratic $h_0 \in C(\mathbb{R}, S[2;2d])$ and sublinear $h_1 \in C(\mathbb{R}, S[1;2d])$. Moreover let $\Theta^y \in \mathcal{C}_{\mathrm{const}}$ and $\Theta^x \in C^1(\mathbb{R}^2, \mathcal{C})$ with $0 < \gamma\,\mathrm{id} \leq \Re\Theta^x(t,s) \leq \gamma'\,\mathrm{id}$ and $\Theta^x(s,s) \in \mathcal{C}_{\mathrm{const}}$ for all $s,t \in]-T,T[$. Then

$$\sup_{-T\leq s,t\leq T}\left\|U^\varepsilon(t,s) - \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; \sum_{n=0}^{N}\varepsilon^n u_n(t,s); \Theta^x(t,s), \Theta^y\right)\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \leq C(T)\varepsilon^{N+1},$$

where $\kappa^{(t,s)}$ and the u_n are uniquely given as

- *the Hamiltonian flow $\kappa^{(t,s)}$ associated to h_0 and*
- *the solutions of*

$$\frac{d}{dt}u_n(t,s,q,p) = u_n(t,s,q,p)\left[\frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)\frac{d}{dt}\mathcal{Z}(t,s,q,p)\right) - ih_1\left(t, X^{\kappa^{(t,s)}}, \Xi^{\kappa^{(t,s)}}\right)\right]$$
$$+ \sum_{k=1}^{n} L_k[h^\varepsilon; \kappa^{(t,s)}; \Theta^x, \Theta^y]u_{n-k}$$

  with initial conditions

$$u_0(s,s,q,p) = \det\left(\Theta^x(s,s) + \Theta^y\right)^{1/2}$$
$$u_n(s,s,q,p) = 0, \qquad n \geq 1,$$

where the $L_k[h^\varepsilon; \kappa^{(t,s)}; \Theta^x, \Theta^y]$ are linear differential operators, whose coefficients depend on $\partial^\alpha h_0$ for $2 \leq |\alpha| \leq 2k$ and $\partial^\alpha h_1$ for $1 \leq |\alpha| \leq 2k-1$.

Proof. By Proposition 4.10, an FIO associated to a C^1 family $\kappa^{(t,s)}$ of canonical transformations of class $\mathcal{B}$ and (x,y)-independent symbol $u = \sum_{n=0}^{N} \varepsilon^n u_n$, $u_n \in C^1(\mathbb{R}, S[0;2d])$ leaves $\mathcal{S}(\mathbb{R}^d,\mathbb{C})$ invariant. Thus we can plug such an operator as an ansatz into the time-dependent Schrödinger equation. By Propositions 7.3 and 7.6 we have a representation

$$\begin{aligned}&\left(i\varepsilon\frac{d}{dt} - \operatorname{op}^\varepsilon(h^\varepsilon)\right)\mathcal{I}^\varepsilon\left(\kappa^{(t,s)};\sum_{n=0}^{N}\varepsilon^n u_n;\Theta^x(t,s),\Theta^y\right)\\ &= \mathcal{I}^\varepsilon\left(\kappa^{(t,s)};\sum_{n=0}^{N+1}\varepsilon^n v_n;\Theta^x(t,s),\Theta^y\right) + \mathcal{R}^\varepsilon\left(\kappa^{(t,s)};v^\varepsilon_{N+2};\Theta^x(t,s),\Theta^y\right)\end{aligned}$$

on $\mathcal{S}(\mathbb{R}^d,\mathbb{C})$, where

$$\left\|\mathcal{R}^\varepsilon\left(\kappa^{(t,s)};v^\varepsilon_{N+2};\Theta^x(t,s),\Theta^y\right)\right\|_{L^2\to L^2} = O(\varepsilon^{N+2}). \tag{8.1}$$

We will show that the $u_n \in S[0,2d]$, $0 \le n \le N$ can be chosen such that the v_n vanish for $0 \le n \le N+1$. Thus, $\mathcal{I}^\varepsilon\left(\kappa^{(t,s)};\sum_{n=0}^{N}\varepsilon^n u_n;\Theta^x(t,s),\Theta^y\right)$ is an asymptotic solution of order $N+2$ and the statement follows from the Magic Lemma 7.2.

In the case $\Theta^x,\Theta^y \in \mathcal{C}_{\text{const}}$, we have the full hierarchy of Propositions 7.3 and 7.6 and see that v_0 is the product of u_0 and

$$\left(-\frac{d}{dt}S^{\kappa^{(t,s)}} + \frac{d}{dt}X^{\kappa^{(t,s)}}\cdot\Xi^{\kappa^{(t,s)}} - h_0\left(t,\kappa^{(t,s)}\right)\right) \tag{8.2}$$

whereas the expressions of Propositions 7.5 and 7.7 for v_0 yield (8.2), when

$$\begin{aligned}&\left(-\frac{d}{dt}S^{\kappa^{(t,s)}} + \frac{d}{dt}X^{\kappa^{(t,s)}}\cdot\Xi^{\kappa^{(t,s)}} - h_0\left(t,\kappa^{(t,s)}\right)\right)\\ &-\frac{1}{2}\left(\frac{d}{dt}\Xi^{\kappa^{(t,s)}} - i\Theta^x(t,s)\frac{d}{dt}X^{\kappa^{(t,s)}}\right)^\dagger\left(x - X^{\kappa^{(t,s)}}(q,p)\right)\\ &+\frac{1}{2}\left(((\partial_x + i\Theta^x(t,s)\partial_\xi)h)\circ\kappa^{(t,s)}\right)(q,p)^\dagger\left(x - X^{\kappa^{(t,s)}}(q,p)\right)\end{aligned}$$

is restricted to $x = X^{\kappa^{(t,s)}}(q,p)$.

As we do not expect $\mathcal{I}^\varepsilon\left(\kappa^{(t,s)};0;\Theta^x(t,s),\Theta^y\right) = 0$ to be a good approximation of $U(t,s)$, we require (8.2) to vanish. Taking derivatives with respect to q and p, we obtain

$$\begin{aligned}&\begin{pmatrix}-\frac{d}{dt}S_q^{\kappa^{(t,s)}} + \left[\frac{d}{dt}X_q^{\kappa^{(t,s)}}\right]\Xi^{\kappa^{(t,s)}} + \Xi_q^{\kappa^{(t,s)}}\left[\frac{d}{dt}X^{\kappa^{(t,s)}}\right]\\ -\frac{d}{dt}S_p^{\kappa^{(t,s)}} + \left[\frac{d}{dt}X_p^{\kappa^{(t,s)}}\right]\Xi^{\kappa^{(t,s)}} + \Xi_p^{\kappa^{(t,s)}}\left[\frac{d}{dt}X^{\kappa^{(t,s)}}\right]\end{pmatrix} - F^{\kappa^{(t,s)}}\nabla_{(x,\xi)}h_0\left(t,\kappa^{(t,s)}\right)\\ &= \begin{pmatrix}-X_q^{\kappa^{(t,s)}}\left[\frac{d}{dt}\Xi^{\kappa^{(t,s)}}\right] + \Xi_q^{\kappa^{(t,s)}}\left[\frac{d}{dt}X^{\kappa^{(t,s)}}\right]\\ -X_p^{\kappa^{(t,s)}}\left[\frac{d}{dt}\Xi^{\kappa^{(t,s)}}\right] + \Xi_p^{\kappa^{(t,s)}}\left[\frac{d}{dt}X^{\kappa^{(t,s)}}\right]\end{pmatrix} - F^{\kappa^{(t,s)}}\nabla_{(x,\xi)}h_0\left(t,\kappa^{(t,s)}\right)\\ &= \begin{pmatrix}\Xi_q^{\kappa^{(t,s)}} & -X_q^{\kappa^{(t,s)}}\\ \Xi_p^{\kappa^{(t,s)}} & -X_p^{\kappa^{(t,s)}}\end{pmatrix}\frac{d}{dt}\kappa^{(t,s)} - F^{\kappa^{(t,s)}}\nabla_{(x,\xi)}h_0\left(t,\kappa^{(t,s)}\right)\\ &= -F^{\kappa^{(t,s)}}J\left(\frac{d}{dt}\kappa^{(t,s)} - J\nabla_{(x,\xi)}h_0\left(t,\kappa^{(t,s)}\right)\right).\end{aligned}$$

Hence we see that a necessary condition for (8.2) $= 0$ is to chose $\kappa^{(t,s)}$ as the Hamiltonian flow associated to h_0. The explicit form

$$S^{\kappa^{(t,s)}}(q,p) = \int_s^t \left[\frac{d}{d\tau} X^{\kappa^{(\tau,s)}}(q,p) \cdot \Xi^{\kappa^{(\tau,s)}}(q,p) - h_0\left(\tau, \kappa^{(\tau,s)}(q,p)\right)\right] d\tau$$

for the action then shows that this condition is also sufficient.

As this choice for $\kappa^{(t,s)}$ implies

$$\frac{d}{dt}\Xi^{\kappa^{(t,s)}}(q,p) - i\Theta^x(t,s)\frac{d}{dt}X^{\kappa^{(t,s)}}(q,p) = -\left[\left(h_x \circ \kappa^{(t,s)}\right)(q,p) + i\Theta^x(t,s)\left(h_\xi \circ \kappa^{(t,s)}\right)(q,p)\right],$$

we obtain

$$\begin{aligned} v_n = {} & i\frac{d}{dt}u_{n-1} - \frac{i}{2}u_{n-1}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)X_z^{\kappa^{(t,s)}}\frac{d}{dt}\Theta^x(t,s)\right) \\ & - u_{n-1}\frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)\left[\partial_z(h_x\circ\kappa^{(t,s)}(q,p)) + i\Theta^x(t,s)\partial_z(h_\xi\circ\kappa^{(t,s)}(q,p))\right]\right) \\ & - \left(h_1\circ\kappa^{(t,s)}\right)(q,p)u_{n-1} + \sum_{k=2}^N L_k[\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]u_{n-k} \\ & - \sum_{k=2}^N L_k[h_0(t);\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]u_{n-k} - \sum_{k=1}^N L_k[h_1(t);\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]u_{n-k-1} \end{aligned}$$

with the convention $u_k = 0, k < 0$, where $L_k[\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]$, $L_k[h_0(t);\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]$ and $L_k[h_0(t);\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]$ are the differential operators of Propositions 7.5 and 7.7.

Recalling that

$$\mathcal{Z}(t,s,q,p) = X_z^{\kappa^{(t,s)}}(q,p)\Theta^x(t,s) + i\Xi_z^{\kappa^{(t,s)}}(q,p),$$

we see

$$\begin{aligned} & -\frac{i}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)X_z^{\kappa^{(t,s)}}(q,p)\frac{d}{dt}\Theta^x(t,s)\right) \\ & \qquad - \frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)\left[\partial_z(h_x\circ\kappa^{(t,s)}(q,p)) + i\Theta^x(t,s)\partial_z(h_\xi\circ\kappa^{(t,s)}(q,p))\right]\right) \\ & = -\frac{i}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)\frac{d}{dt}\mathcal{Z}(t,s,q,p)\right) \end{aligned}$$

and thus

$$\begin{aligned} v_n = {} & i\frac{d}{dt}u_{n-1} - i\left[\frac{1}{2}\mathrm{tr}\left(\mathcal{Z}^{-1}(t,s,q,p)\frac{d}{dt}\mathcal{Z}(t,s,q,p)\right)u_0 - i\left(h_1\circ\kappa^{(t,s)}\right)(q,p)\right]u_{n-1} \\ & + \sum_{k=2}^N L_k[h^\varepsilon;\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]u_{n-k}, \end{aligned}$$

where we set

$$\begin{aligned} L_k[\kappa^{(t,s)};h^\varepsilon;\Theta^x(t,s),\Theta^y] := {} & L_k[\kappa^{(t,s)};\Theta^x(t,s),\Theta^y] \\ & - L'_k[h_0;\kappa^{(t,s)};\Theta^x(t,s),\Theta^y] - L'_{k-1}[h_1;\kappa^{(t,s)};\Theta^x(t,s),\Theta^y]. \end{aligned}$$

As the linearisation of $\det(A)$ for invertible A is $\det(A)\mathrm{tr}(A^{-1}\mathrm{d}A)$, the equations $v_n = 0$ have the solutions

$$u_0(t,s,q,p) = C_0 \left(\det(\mathcal{Z}(t,s,q,p))\right)^{\frac{1}{2}} \exp\left[-i\int_s^t h_1\left(\tau, \kappa^{(\tau,s)}\right) d\tau\right] \qquad \text{and}$$

$$u_n(t,s,q,p) = u_0(t,s,q,p) \exp\left[-\int_s^t \sum_{k=1}^N L_{k+1}[\kappa^{(t,s)}; h^\varepsilon(\tau); \Theta^x(\tau,s), \Theta^y] u_{n-k}(\tau,s,q,p) d\tau\right],$$

which are of class $S[0;2d]$ due to the assumptions on h^ε. The correct choice for the constant C_0 to obtain

$$\mathcal{I}^\varepsilon\left(\mathrm{id}; \sum_{n=0}^N \varepsilon^n u_n(s,s); \Theta^x(s,s), \Theta^y\right) = \mathrm{id}$$

follows from Proposition 4.13.

It remains to show the uniqueness. Assume that there are $\widetilde{\kappa}^{(t,s)}$ and $\widetilde{u} \in S[0;2d]$ such that

$$\left\|U^\varepsilon(t,s) - \mathcal{I}^\varepsilon\left(\widetilde{\kappa}^{(t,s)}; \widetilde{u}; \Theta^x(t), \Theta^y\right)\right\| \leq C'(T)\varepsilon.$$

In this case we have

$$\left\|\mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_0; \Theta^x(t), \Theta^y\right) - \mathcal{I}^\varepsilon\left(\widetilde{\kappa}^{(t,s)}; \widetilde{u}; \Theta^x(t), \Theta^y\right)\right\| \leq \left(C(T) + C'(T)\right)\varepsilon$$

and hence

$$\begin{aligned}&\lim_{\varepsilon\to 0}\left\langle g^{\varepsilon,\overline{\Theta^x(t,s)}(t,q_0,p_0)}_{\kappa^{(t,s)}(q_0,p_0)} \middle| \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_0; \Theta^x(t,s), \Theta^y\right) g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle_{L^2(\mathbb{R}^d)} \\ &= \lim_{\varepsilon\to 0}\left\langle g^{\varepsilon,\overline{\Theta^x(t,s)}(t,q_0,p_0)}_{\kappa^{(t,s)}(q_0,p_0)} \middle| \mathcal{I}^\varepsilon\left(\widetilde{\kappa}^{(t,s)}; \widetilde{u}; \Theta^x(t,s), \Theta^y\right) g^{\varepsilon,\Theta^y(q_0,p_0)}_{(q_0,p_0)}\right\rangle_{L^2(\mathbb{R}^d)},\end{aligned}$$

so Proposition 4.13 shows that $\widetilde{\kappa}^{(t,s)} = \kappa^{(t,s)}$ and $\widetilde{u} = u_0$ on $\mathrm{supp}(u_0) = \mathbb{R}^{2d}$. The uniqueness of the higher order symbols follows analogously. □

Corollary 7.8 and the form of u_0 yield the following result for the Ehrenfest timescale.

8.2 Corollary (Ehrenfest-timescale)**.** *In the situation of Theorem 8.1 and under the additional assumption*

$$\sup_{(t,x,\xi)\in\mathbb{R}^{2d+1}} \left\|\partial^\alpha_{(x,\xi)} \mathrm{Hess}_{(x,\xi)} h(t,x,\xi)\right\| < \infty.$$

for all $\alpha \in \mathbb{N}$, we have the following bound for the Ehrenfest timescale $T(\varepsilon) = C_T \log(\varepsilon^{-1})$:

$$\sup_{-T(\varepsilon)\leq s,t\leq T(\varepsilon)} \left\|U^\varepsilon(t,s) - \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_0; \Theta^x, \Theta^y\right)\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \leq C(\rho)\varepsilon^{1-\rho},$$

where ρ can be made arbitrary small if C_T chosen small enough.

As the Initial Value Representations are uniformly close to unitary operators they approximately inherit some properties.

8.3 Corollary. *Consider the situation of Theorem 8.1 and let* $u_N = \sum_{n=0}^{N} \varepsilon^n u_n$.

- *The Initial Value Representations are almost unitary, i.e. they fulfill*

$$\left\| \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x(t,s), \Theta^y\right) \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x(t,s), \Theta^y\right)^* - \mathrm{id} \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C\varepsilon^{N+1}$$

$$\left\| \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x(t,s), \Theta^y\right)^* \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x(t,s), \Theta^y\right) - \mathrm{id} \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C\varepsilon^{N+1}$$

- *The Initial Value Representations almost fulfill the group property*

$$\Big\| \mathcal{I}^\varepsilon\left(\kappa^{(t,t')}; u_N; \Theta^x(t,t'), \Theta^y\right) \mathcal{I}^\varepsilon\left(\kappa^{(t',s)}; u_N; \Theta^x(t',s), \Theta^y\right) - \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x(t,s), \Theta^y\right) \Big\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C\varepsilon^{N+1}$$

We also get an simple Egorov result for $a \in S[0; 2d]$, namely

$$\left\| \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x, \Theta^y\right)^* \mathrm{op}^\varepsilon(a) \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u_N; \Theta^x, \Theta^y\right) - \mathrm{op}^\varepsilon(a \circ \kappa^{(t,s)}) \right\| \le C\varepsilon \tag{8.3}$$

if we use the classical Egorov Theorem, see e.g. Théorème IV-10 in [Rob87].

8.4 Theorem (Egorov)**.** *Let* $a \in S[2; 2d]$ *be subquadratic and* $h(t) \in C(\mathbb{R}, S[+\infty; 2d])$ *such that* $\mathrm{op}^\varepsilon(h(t))$ *generates a unique unitary time-evolution* $U^\varepsilon(t,s)$*. Then*

$$\left\| U^\varepsilon(s,t)\mathrm{op}^\varepsilon(a)U^\varepsilon(t,s) - \mathrm{op}^\varepsilon\left(a \circ \kappa^t\right) \right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C\varepsilon^2,$$

where $\kappa^{(t,s)}$ *is the flow associated to* $h(t)$ *and the* C *depends on* $\partial^\alpha h$ *and* $\partial^\alpha a$ *for* $|\alpha| \ge 3$.

In view of Theorem 8.4 the restriction to $a \in S[0; 2d]$ in (8.3) is not satisfactory. Indeed, (8.3) is not the strongest result one can obtain from the theory we developed. Combining Corollary 4.19 on the form of formal adjoints of Fourier Integral Operators with the composition result Proposition 7.5, we can at least allow for sublinear observables, whereas subquadratic observables do not seem to be accessible in the context of $L^2(\mathbb{R}^d)$-boundedness.

8.5 Proposition. *Let* κ *a canonical transformation of class* $\mathcal{B}$, $\Theta^x, \Theta^y \in \mathcal{C}$ $u \in S[0; 2d]$*. If* $a \in S[1; 2d]$ *is sublinear, we have*

$$\|\mathrm{op}^\varepsilon(a)\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y) - \mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)\, \mathrm{op}^\varepsilon\left(a \circ \kappa\right)\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \le C\varepsilon. \tag{8.4}$$

The assumption on sublinearity of the symbol a is in accordance with a corresponding result in [Tat04]. Note that neither the canonical transformation has to arise from a Hamiltonian flow nor do not require the FIO to be an Initial Value Representation but that the result holds for arbitrary canonical transformations κ and symbols $u \in S[0; 2d]$. Unfortunately, we have no general result on the almost unitarity of our FIOs, which forces us to present the Egorov result in the form (8.4). If it is known that the canonical transformation κ arises from a subquadratic Hamiltonian, we can turn (8.3) into the traditional form (8.4) with help of Corollary 8.3.

We address one last topic, namely the relation between Initial Value Representations and quadratic Hamiltonians, which yield linear canonical transformations and thus q and p independent $F^{\kappa^{(t,s)}}$ and u_0. From its construction, it is clear that the TGA is exact in this case. Also the Herman-Kluk propagator equals $U(t,s)$ due to the form of the symbols v_2 in Propositions 7.3 and 7.6. For arbitrary $\Theta^x, \Theta^y \in \mathcal{C}$, these symbols will in general not vanish. Moreover, Proposition 4.13 suggests that a symbol, which recovers the identity in terms of a general FIO has to be x-dependent. As the propagator of the harmonic oscillator equals the identity after every second oscillation period, one can thus not expect that general IVRs are exact for quadratic Hamiltonians.

8.2 Two special cases

Theorem 8.1 gives rise to an infinite number of Initial Value Representations. The question, which choice of Θ^x and Θ^y gives the best method cannot be answered on the basis of the suboptimal estimate of Theorem 5.4, compare the discussion after Proposition 4.13. However, there are two choices for Θ^x and Θ^y, which are immediate and were already mentioned several times, namely $\Theta^x, \Theta^y \in \mathcal{C}_{\text{const}}$, which yields the Herman-Kluk propagator and $\Theta^x(t,s) = \Theta_{\text{TGA}}$, which yields the Thawed Gaussian IVR, compare (6.4).

It remains to show that the TGA is covered by Theorem 8.1:

8.6 Lemma. $\Theta_{\text{TGA}}(t,s,q,p)$ *is symmetric, belongs to* $S[0;2d]$ *and fulfills*

$$\langle x, \Re\Theta_{\text{TGA}} x\rangle_{\mathbb{R}^d} \geq C(t)\left\|x\right\|^2,$$

uniformly in $(q,p) \in \mathbb{R}^{2d}$*, where* $C(t) > 0$ *behaves like* $C\varepsilon^\rho$ *in the Ehrenfest case. Moreover, the principal symbol* u_0 *may be expressed in the well-known form*

$$u_{\text{TGA}}(t,s,q,p) = 2^{-d/2}\left(\det\left(X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right)\right)^{-\frac{1}{2}}.$$

Proof. $\Theta_{\text{TGA}}(t,s,q,p)$ is symmetric, as

$$\left[\Xi_q^{\kappa^{(t,s)}} + i\Xi_p^{\kappa^{(t,s)}}\right]\left[\left(X_q^{\kappa^{(t,s)}}\right)^\dagger + i\left(X_p^{\kappa^{(t,s)}}\right)^\dagger\right] = \left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]\left[\left(\Xi_q^{\kappa^{(t,s)}}\right)^\dagger + i\left(\Xi_p^{\kappa^{(t,s)}}\right)^\dagger\right]$$

by the symplecticity of $F^{\kappa^{(t,s)}}$. Moreover, it has positive definite real part:

$$\begin{aligned}2\Re\Theta^x(t,q,p) = &-i\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]^{-1}\left[\Xi_q^{\kappa^{(t,s)}} + i\Xi_p^{\kappa^{(t,s)}}\right] \\ &+ i\left[\left(\Xi_q^{\kappa^{(t,s)}}\right)^\dagger - i\left(\Xi_p^{\kappa^{(t,s)}}\right)^\dagger\right]\left[\left(X_q^{\kappa^{(t,s)}}\right)^\dagger - i\left(X_p^{\kappa^{(t,s)}}\right)^\dagger\right]^{-1}\end{aligned}$$

and thus

$$\begin{aligned}&2\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]\Re\Theta^x(t,q,p)\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]^* \\ &= -i\left[\Xi_q^{\kappa^{(t,s)}} + i\Xi_p^{\kappa^{(t,s)}}\right]\left[\left(X_q^{\kappa^{(t,s)}}\right)^\dagger - i\left(X_p^{\kappa^{(t,s)}}\right)^\dagger\right] \\ &\quad + i\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]\left[\left(\Xi_q^{\kappa^{(t,s)}}\right)^\dagger - i\left(\Xi_p^{\kappa^{(t,s)}}\right)^\dagger\right] \\ &= -\Xi_q^{\kappa^{(t,s)}}\left(X_p^{\kappa^{(t,s)}}\right)^\dagger + \Xi_p^{\kappa^{(t,s)}}\left(X_q^{\kappa^{(t,s)}}\right)^\dagger - i\Xi_q^{\kappa^{(t,s)}}\left(X_q^{\kappa^{(t,s)}}\right)^\dagger - i\Xi_p^{\kappa^{(t,s)}}\left(X_p^{\kappa^{(t,s)}}\right)^\dagger \\ &\quad + X_q^{\kappa^{(t,s)}}\left(\Xi_p^{\kappa^{(t,s)}}\right)^\dagger - X_p^{\kappa^{(t,s)}}\left(\Xi_q^{\kappa^{(t,s)}}\right)^\dagger + iX_q^{\kappa^{(t,s)}}\left(\Xi_q^{\kappa^{(t,s)}}\right)^\dagger + iX_p^{\kappa^{(t,s)}}\left(\Xi_p^{\kappa^{(t,s)}}\right)^\dagger \\ &= 2\mathrm{id}\end{aligned}$$

Hence, for $x \in \mathbb{R}^d$

$$\begin{aligned}\langle x, \Re\Theta^x x\rangle_{\mathbb{R}^d} = \langle x, \Re\Theta^x x\rangle_{\mathbb{C}^d} &= \left\langle\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]^{-1} x, \left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]^{-1} x\right\rangle_{\mathbb{C}^d} \\ &= \left\|\left[X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right]^{-1} x\right\|^2 \\ &\geq \left\|X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right\|^{-2}\left\|x\right\|^2.\end{aligned}$$

As $\kappa^{(t,s)}$ is of class $\mathcal{B}$, $\left\| X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}} \right\|_{L^\infty(\mathbb{R}^{2d})} \leq C(t)$ and thus $\langle x, \Re\Theta^x x\rangle_{\mathbb{R}^d} \geq C(t)^{-2} \|x\|^2$.

For the symbol class of Θ_{TGA} we recall the expression of a matrix inverse by the formula of minors

$$\Theta^{-1}(q,p) = \frac{1}{\det\Theta(q,p)} \begin{pmatrix} \Theta_{11}(q,p) & -\Theta_{21}(q,p) & \dots & (-1)^{d+1}\Theta_{d1}(q,p) \\ -\Theta_{12}(q,p) & \Theta_{22}(q,p) & \dots & (-1)^{d+2}\Theta_{d2}(q,p) \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{d+1}\Theta_{1d}(q,p) & (-1)^{d+2}\Theta_{2d}(q,p) & \dots & \Theta_{dd}(q,p) \end{pmatrix},$$

which we apply to $\Theta = X_q^{\kappa^{(t,s)}}(q,p) + iX_p^{\kappa^{(t,s)}}(q,p)$. Because of the form of Θ_{TGA} and the fact that $\kappa^{(t,s)}$ is of class $\mathcal{B}$, it is enough to show a bound away from zero for $\det\left(X_q^{\kappa^{(t,s)}}(q,p) + iX_p^{\kappa^{(t,s)}}(q,p)\right)$. But as $\langle x, \Re\Theta^x x\rangle_{\mathbb{R}^d} \geq C(t)^{-2}\|x\|^2$, the real parts of the eigenvalues are bounded away from zero and with them the determinant.

By the uniqueness of the symbol u_0 and the results of [BR01], it is clear that

$$u_0(t,s,q,p) = \left(\det\left(X_q^{\kappa^{(t,s)}}(q,p)\Theta_{\mathrm{TGA}} - iX_p^{\kappa^{(t,s)}}(q,p)\Theta_{\mathrm{TGA}} + i\Xi^{\kappa^{(t,s)}}(q,p) + \Xi_p^{\kappa^{(t,s)}}(q,p)\right)\right)^{\frac{1}{2}}$$

may be cast in the claimed form.

However, this also follows directly from the symplecticity of $F^{\kappa^{(t,s)}}(q,p)$ as

$$-i\left(X_q^{\kappa^{(t,s)}} - iX_p^{\kappa^{(t,s)}}\right)\left(\Xi_q^{\kappa^{(t,s)}} + i\Xi_p^{\kappa^{(t,s)}}\right)^\dagger + i\left(\Xi_q^{\kappa^{(t,s)}} - i\Xi_p^{\kappa^{(t,s)}}\right)\left(X_q^{\kappa^{(t,s)}} + iX_p^{\kappa^{(t,s)}}\right)^\dagger = 2\mathrm{id}.$$

□

8.3 Some numerical results

We close the dissertation by some numerical experiments on IVRs. The major challenge for the implementation is the discretization of the oscillatory phase-space integral. As the quadrature of such expressions is far beyond the scope of this work, we restrict to one-dimensional problems, where grid-based approaches are feasible.

Moreover, treat Hamiltonians of the classical Schrödinger form

$$i\varepsilon \frac{d}{dt}\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V(x)\psi \qquad \psi(0) = \psi_0(t),$$

which allows to obtain a reference solution by the numerically well understood Strang splitting method [Str68] with Fourier differencing, see [JL00]. The parameters and accuracy of the reference solutions are collected in the appendix.

We will study three IVRs, namely the Thawed Gaussian IVR, the Herman-Kluk propagator and the first correction of the Herman-Kluk propagator. Calculations based on the proof of Proposition 7.3 show that the first correction has the symbol

$$u_0(t,s,q,p)\left[1 + \varepsilon \exp\left(-i\int_s^t (L_2 u_0)(\tau,s,q,p)\,d\tau\right)\right],$$

where

$$\begin{aligned} L_2 u_0(t,s,q,p) = &- \frac{5\mathcal{Z}_z^2(q,p)}{8\mathcal{Z}^4(q,p)} u_0(t,s,q,p) + \frac{\mathcal{Z}_z(q,p)}{4\mathcal{Z}^3(q,p)}\left[V''\left(X^{\kappa^{(t,s)}}(q,p)\right) - 1\right] u_0(t,s,q,p) \\ &+ \left[\frac{5\mathcal{Z}_z(q,p) X_z^{\kappa^{(t,s)}}(q,p)}{12\mathcal{Z}^3(q,p)} - \frac{X_{zz}^{\kappa^{(t,s)}}(q,p)}{6\mathcal{Z}_z^2(q,p)}\right] V^{(3)}\left(X^{\kappa^{(t,s)}}(q,p)\right) u_0(t,s,q,p) \\ &- \frac{1}{8}\frac{\left(X_z^{\kappa^{(t,s)}}(q,p)\right)^2}{\mathcal{Z}^2(q,p)} V^{(4)}\left(X^{\kappa^{(t,s)}}(q,p)\right) u_0(t,s,q,p), \end{aligned}$$

compare also [HK06].

We study three potentials

$V(x) = x^2/2$ The harmonic oscillator is the traditional starting point for all semiclassical methods. As the treated IVRs are exact for this case, this section is more concerned with issues of the implementation than with actual approximation properties of IVRs.

$V(x) = (1 - e^{-x})^2$ The Morse potential is used to model the single-state dynamics of diatomic molecules. Around the minimum, it only shows a mild anharmonicity.

$V(x) = x^4/4$ Finally, we treat the quartic oscillator which shows a stronger anharmonicity.

The initial datum is chosen as the coherent state centered at $(1,0)$ in phase space for all computations, i.e.

$$\psi_0(x) = g^{\varepsilon}_{(1,0)} = (\pi\varepsilon)^{-1/4} e^{-(x-1)^2/2\varepsilon}$$

and the time-interval under consideration is [0,25].

8.3.1 The harmonic oscillator

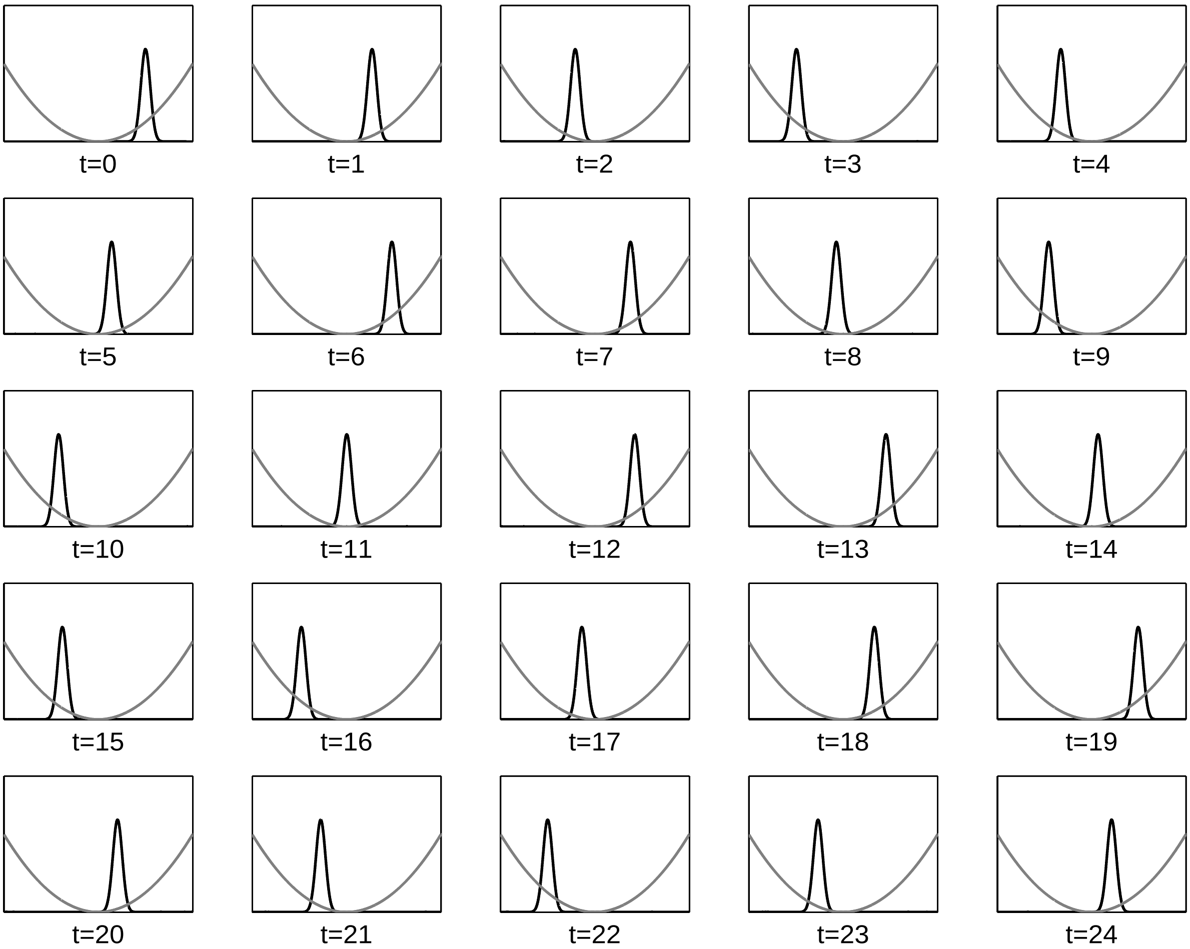

Figure 8.1: Propagation of the initial datum in the harmonic oscillator. The potential is shown by the grey line.

We start our discussion with the harmonic oscillator. As mentioned after Theorem 8.1, both the Herman-Kluk propagator and the Thawed Gaussian IVR are exact in this case. To give the reader an idea about the length of the time-interval, the propagation for $\varepsilon = 0.01$ is shown in Figure 8.1. One can see that the wavepacket completes four full oscillations.

As already mentioned, we chose a grid based approach for the discretization. More precisely, using the Matlab colon notation, our grids are given by

$$(1,0) + G_{kl}\left(\frac{\varepsilon}{0.1}\right)^{\frac{1}{2}}, \text{ where } G_{kl} := [-2 : 0.1\cdot 2^k : 2] \times [-2 : 0.1\cdot 2^l : 2] \subset \mathbb{R}^{2d},$$

i.e. we have a full grid G_{00} with 1681 points and coarsening parameters k, l such that G_{kl} has $1680/2^{k+l} + 1$ points.

k/l	0	1	2
0	1.45e-7	1.10e-7	2.96e-3
1	1.10e-7	5.57e-8	2.96e-3
2	2.96e-3	2.96e-3	4.19e-3

Table 8.1: Dependence of the initial sampling error on the grid in L^2-norm.

Table 8.1 collects the error of the initial sampling for different numbers of sampling points. Note that an error of 1e-8 corresponds to machine precision, as it is actually

$$\left\| U(t,s)\psi_0 - \mathcal{I}^\varepsilon\left(\kappa^{(t,s)}; u; \Theta^x, \Theta^y\right)\psi_0 \right\|_{L^2}^2$$

which is computed. The somewhat strange behavior that a higher number of sampling point leads to a larger error has to be attributed to floating point arithmetics. As the sampling error is close to machine precision, the roundoff errors gain importance. As higher number of sampling points require more basic algebraic manipulations for the reconstruction of the wavefunction, it is this error which is more pronounced on fine grids.

We turn to the significance of the width parameters Θ^x and Θ^y. Table 8.2 lists the error for different values of the equally chosen matrices. It turns out that the smallest error is achieved for the width of the initial datum but also that the sampling is rather robust on fine grids.

$k, l/\Theta^x, \Theta^y$	0.25	0.5	0.75	1	1.25	1.5	1.75
k=l=0	1.39e-4	3.64e-6	4.24e-7	1.45e-7	3.07e-7	7.81e-7	1.77e-6
k=l=1	2.31e-3	5.45e-6	1.83e-7	5.57e-8	1.29e-7	3.65e-7	1.31e-6
k=l=2	3.02e-1	6.47e-2	1.39e-2	4.19e-3	1.02e-2	2.32e-2	4.17e-2

Table 8.2: Dependence of sampling error on the width matrix in L^2-norm.

When it comes to the propagation, ordinary differential equations have to be solved. For this, we rely on the well-established method DOPRI5(4) of Dormand and Prince [DP80]. A pitfall here is the appropriate choice of the tolerance for the method. Due to the oscillatory structure even small errors of the classical quantities lead to large overall errors. More precisely, if the method computes for example $S^{\kappa^{(t,s)}}_{\mathrm{DOPRI}}(q,p) = S^{\kappa^{(t,s)}}(q,p) + \delta$ with $\delta = O(\varepsilon)$, we have

$$e^{iS^{\kappa^{(t,s)}}_{\mathrm{DOPRI}}(q,p)/\varepsilon} - e^{iS^{\kappa^{(t,s)}}(q,p)/\varepsilon} = e^{i\delta/\varepsilon} = O(1).$$

Table 8.3 collects the errors at the final time $t = 25$. The larger error for big ε reflects the tolerance, which is chosen as $\mathrm{TOL_{rel}} = 10^{-3}\varepsilon^2$ and $\mathrm{TOL_{abs}} = 10^{-4}\varepsilon^2$.

One should be aware that a well-chosen initial sampling and a strict tolerance to the ODE-solver are not sufficient to control the error of the IVRs. This is the message of Figure 8.2,

ε	1	1e-1	1e-2	1e-3	1e-4
Error	1.87e-3	3.41e-5	5.04e-7	1.96e-6	5.01e-6

Table 8.3: Error of the Herman-Kluk solution at $t = 25$.

which shows the error of the Herman-Kluk propagation and the TGA-IVR over time for different values of the initial width Θ^y. As the approximate evolution of Gaussians used in the TGA is exact for the harmonic oscillator, its error is constant over time. On the other hand, the error of the Herman-Kluk propagator goes up and down in time with the oscillations of the wavepacket. Though the error is always dominated by the initial sampling error, one will in general be confronted with the opposite behavior as we will see later on.

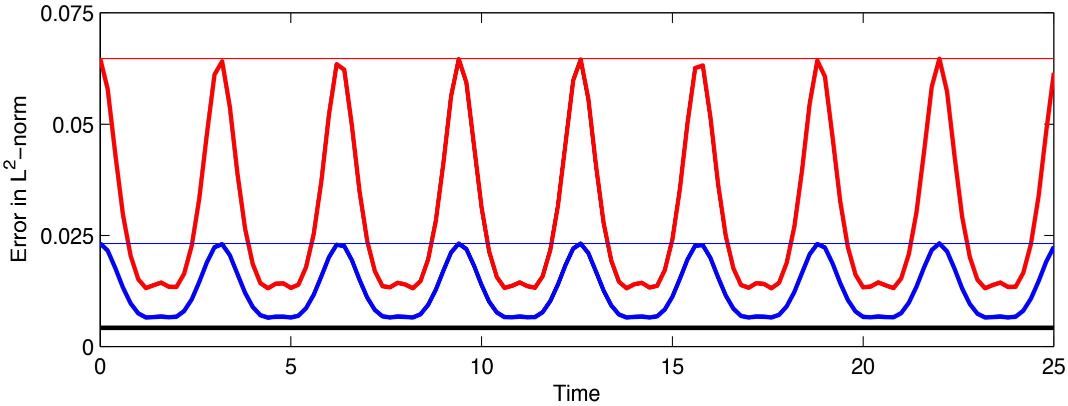

Figure 8.2: Error of the Herman-Kluk method (thick lines) and the Thawed Gaussian IVR (thin lines) over time for the $\varepsilon = 0.01$ and $k = l = 2$. The two black lines correspond to $\Theta^y = 1$ and are thus identic, whereas $\Theta^y = 0.5$ was used for the red lines and $\Theta^y = 1.5$ yields the blue lines.

8.3.2 The Morse potential

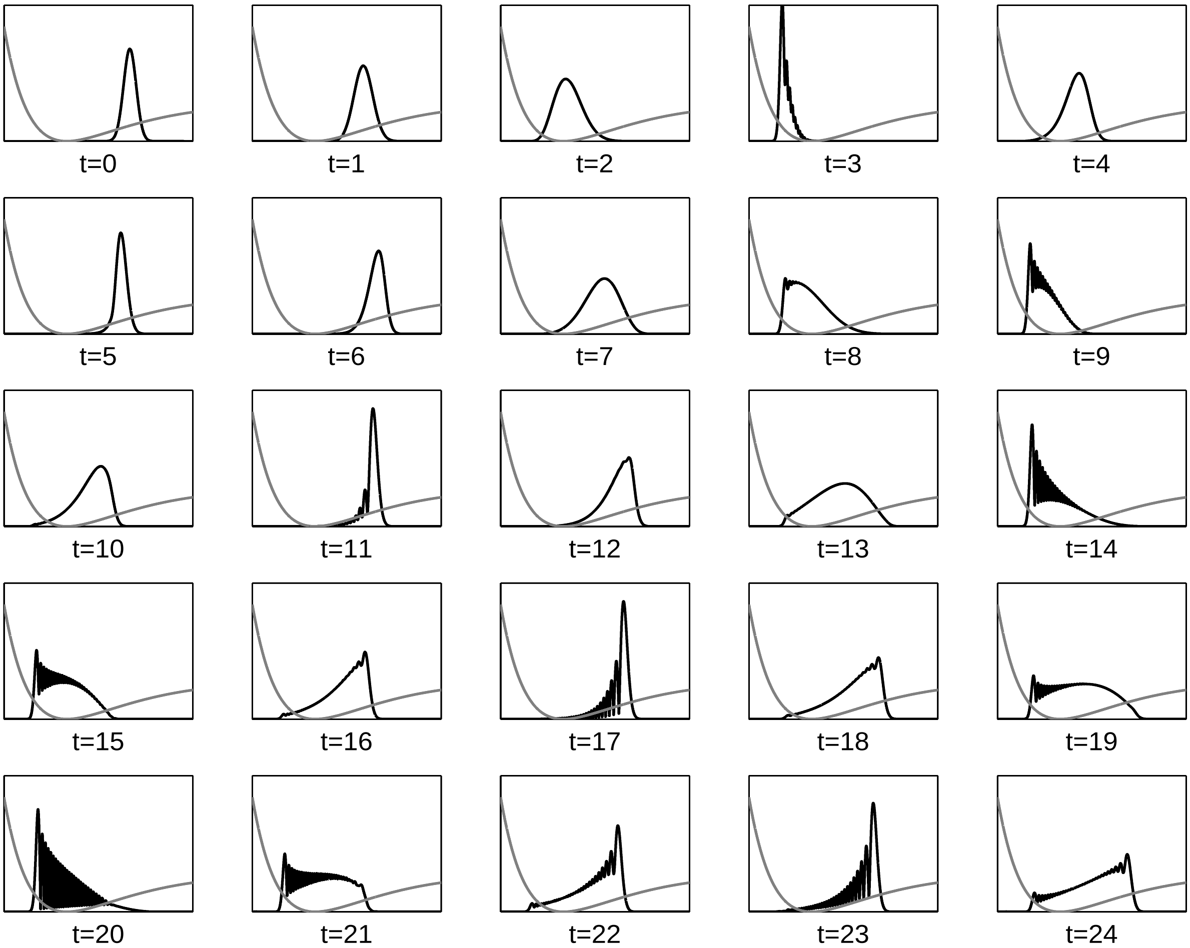

Figure 8.3: Propagation of the initial datum in the Morse potential

We turn to a more interesting problem, namely the Morse potential, which is given by

$$V(x) = (1 - e^{-x})^2.$$

The Morse potential is used to model the single state dynamics in diatomic molecules in Born-Oppenheimer approximation. The physically relevant regime for ε is between 0.001 and 0.01. Figure 8.3 shows the propagation of the initial datum for $\varepsilon = 0.01$. One can see that oscillations in the solution arise from the exponential growth of the potential on the left side.

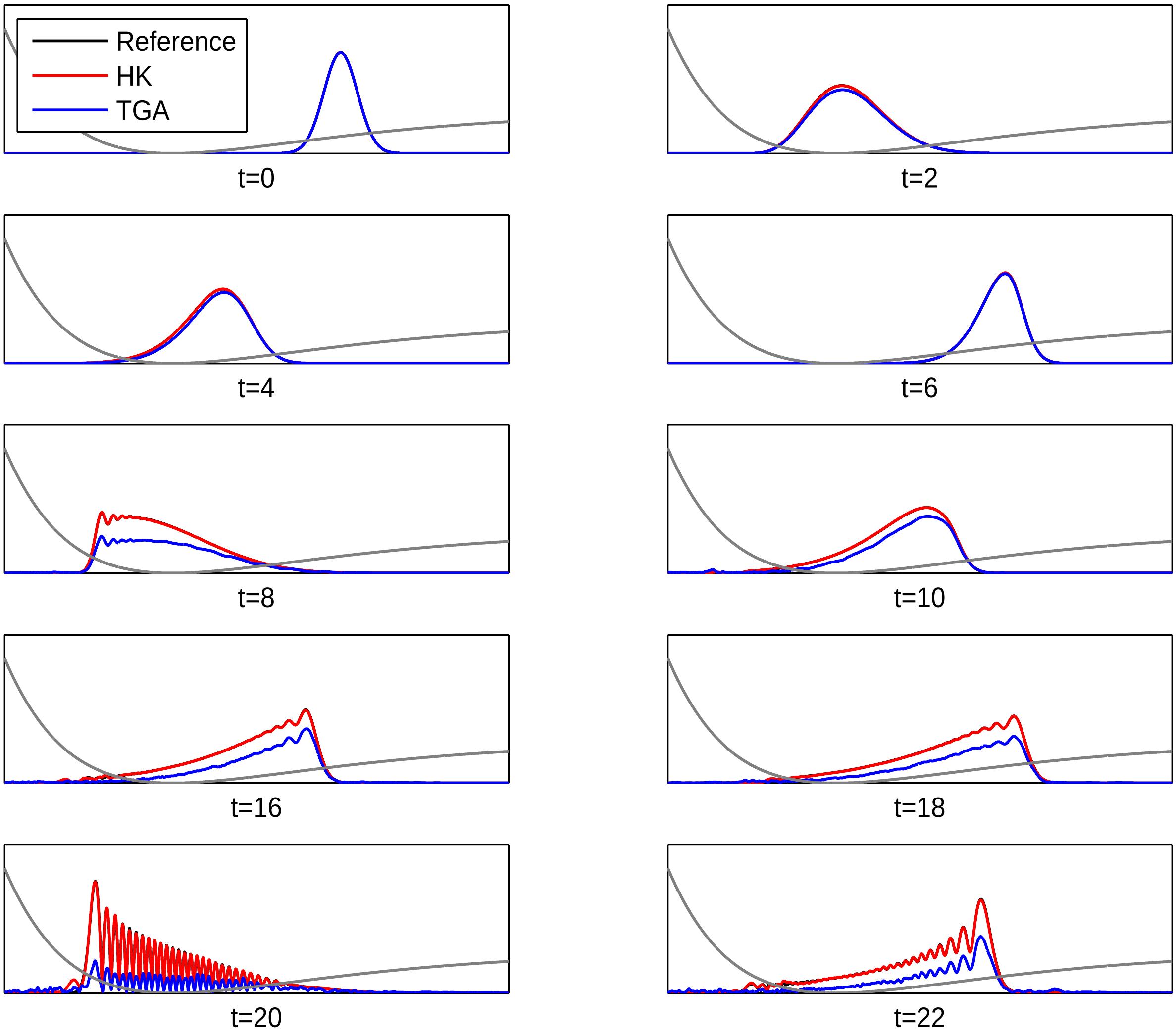

Figure 8.4: Propagation of the initial datum in the Morse potential by the IVRs.

Figure 8.4 compares the Herman-Kluk propagator and the TGA for $\varepsilon = 0.01$. Whereas the TGA loses a significant amount of the total mass, the quality of the Herman-Kluk solution, which covers the reference solution in almost all of the plots, is impressive.

For a more quantitative assessment, we turn to Figure 8.5, which shows the error of the various methods over time. There are two interesting messages concerning the Herman-Kluk propagator. First, comparing the blue and the black lines, one sees that the initial sampling is not sufficient to control the quality of the approximation. Although the coarser grid shows a smaller initial sampling error, compare Table 8.1, it yields a much larger error of the propagation. Second, one sees that the first correction of the Herman-Kluk propagator actually reduces the error in the short-time regime, but that its long term error is larger than that of the lowest-order method.

Figure 8.6 depicts the behaviour of the L^2-error at $t = 10$ for $\varepsilon \in$[1e-4,1e-1]. Both the HK and the TGA error show the perfect $O(\varepsilon)$ asymptotic predicted by Theorem 8.1. On the other hand, the $O(\varepsilon^2)$ asymptotic of the first correction of the Herman-Kluk propagator is not seen in the

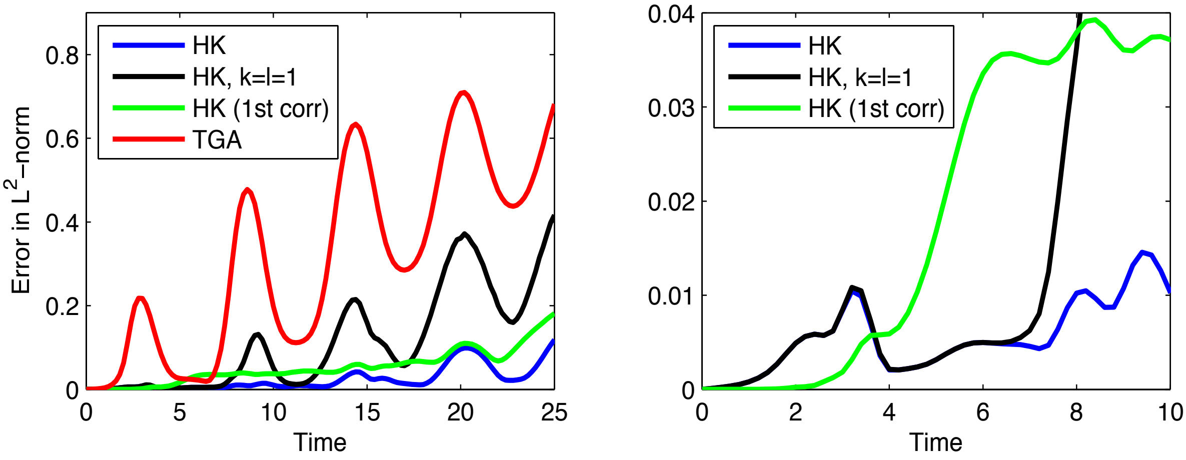

Figure 8.5: L^2-error of the IVRs for the Morse potential and $\varepsilon = 0.01$.

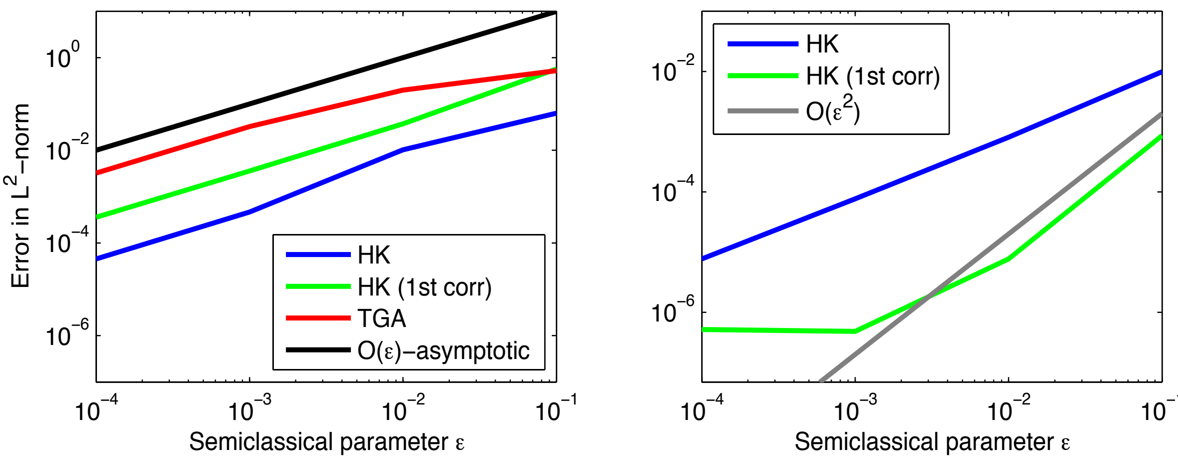

Figure 8.6: Asymptotic behaviour of the L^2-error for the Morse potential at $t = 10$ and $t = 1$.

figure. This is due to numerical difficulties. As explained before, due to our choice of tolerances the integrand is approximated by the ODE solver with an error $O(\varepsilon)$, thus the numerical error is dominating the methodical error in this case. However, pushing the computation to higher accuracy is a serious challenge. By a rule of thumb, the borderline for the accuracy of ODE solvers is the square root of the machine precision, i.e. around 1e-8, so an accuracy of $O(\varepsilon^3)$, which one would need is not obtainable for small ε. This also applies to the reference solution, whose quality does not improve, when more gridpoints and timesteps are added.

However, if one restricts to short times, i.e. to $t = 1$ as in the right plot of Figure 8.6, the numerical errors are small enough to show an $O(\varepsilon^2)$ asymptotic at least for large ε.

8.3.3 The quartic oscillator

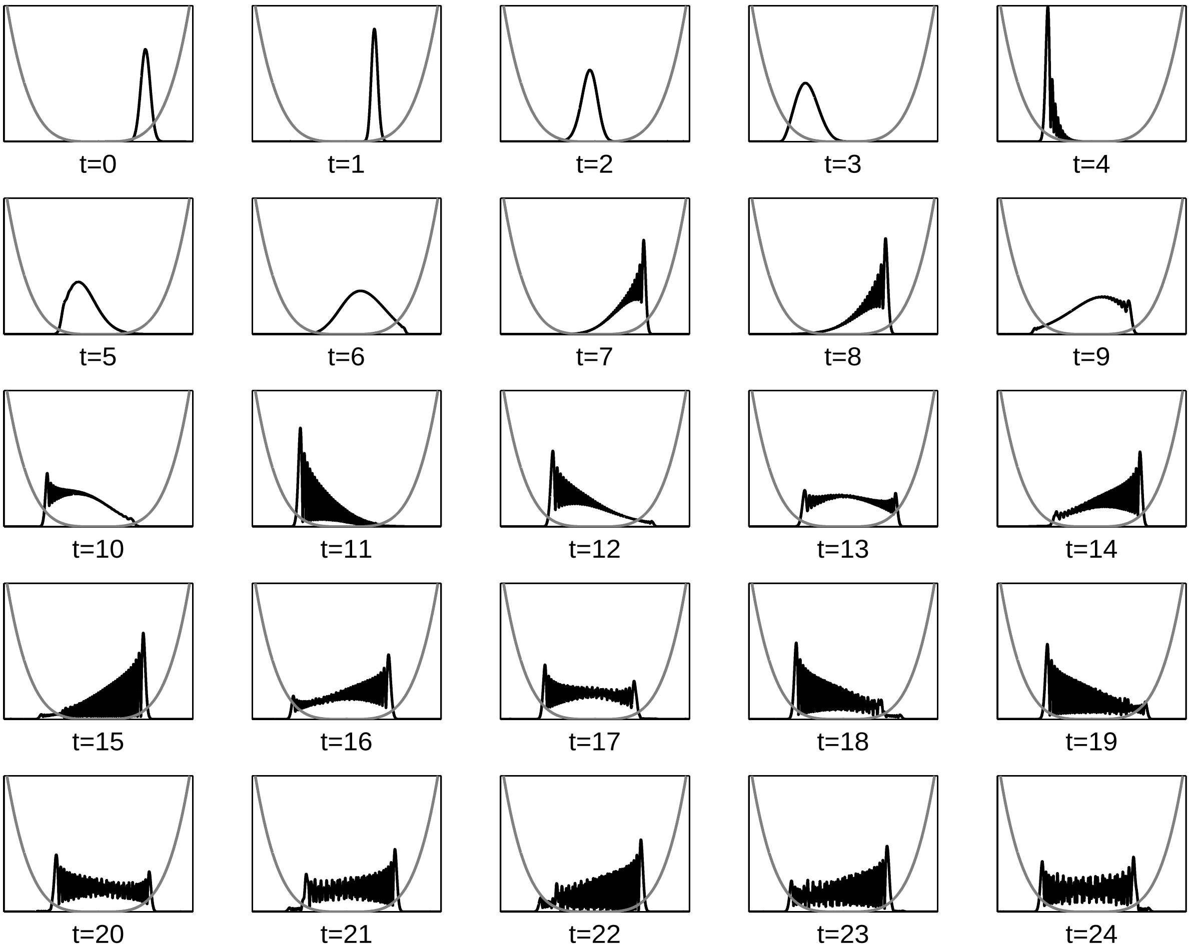

Figure 8.7: Propagation of the initial datum in the quartic oscillator.

As last example we consider the quartic oscillator $V(x) = x^4/4$. As one can see from Figure 8.7 the solution develops even stronger oscillations in this case.

Again the Herman-Kluk solution shows an impressive quality, see Figure 8.8 as long as the oscillations of the solution are not too strong, whereas the TGA-solution deteriorates quickly.

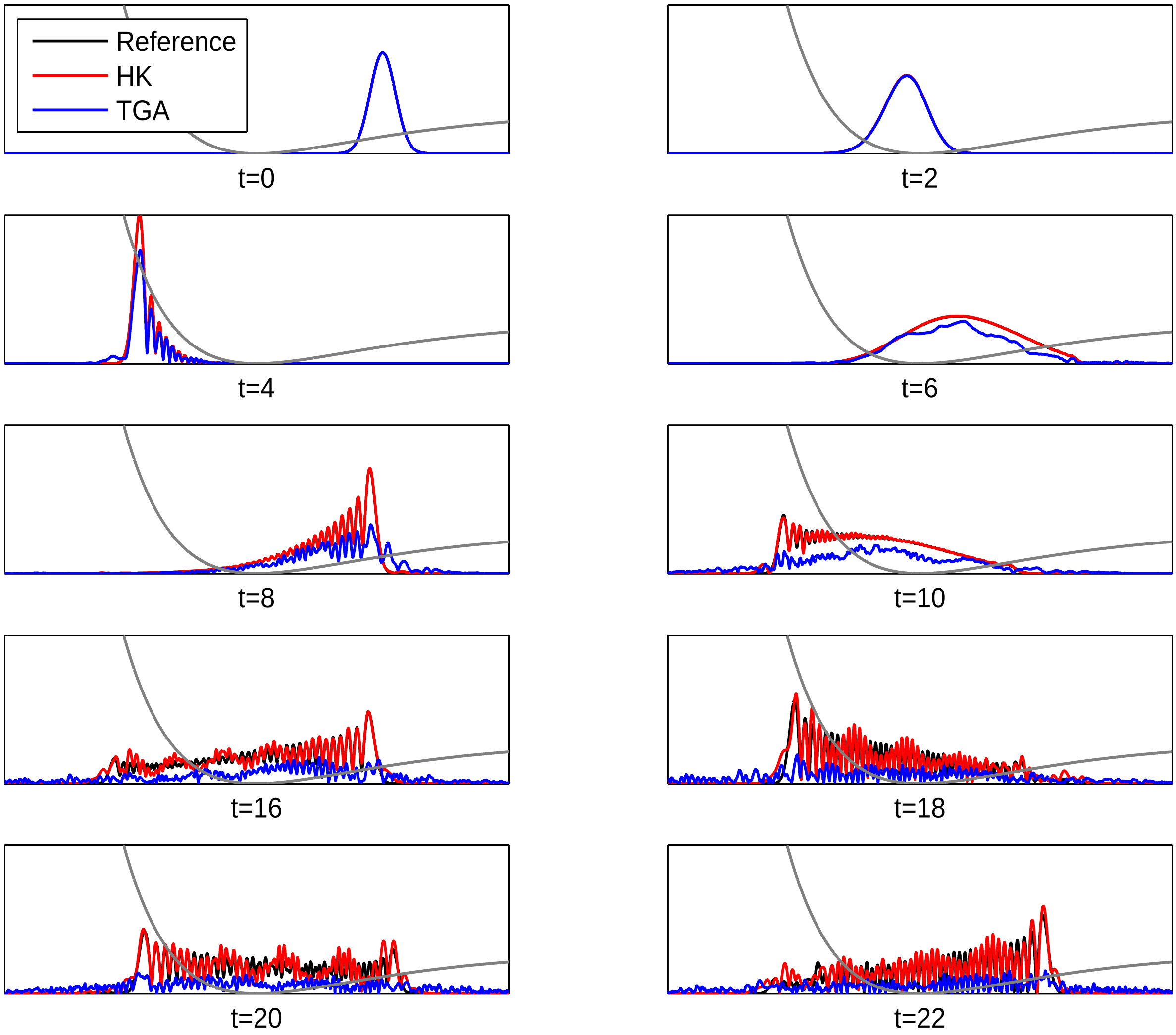

Figure 8.8: Propagation of the initial datum in the quartic oscillator by the IVRs.

Also the behaviour of the error is similar to the case of the Morse oscillator, see Figure 8.9. A difference lies in the fact that the first correction stays closer to the Herman-Kluk solution over time. With respect to the asymptotic behaviour of the error, one recognises again a perfect $O(\varepsilon)$ behaviour in the regime $\varepsilon \in$[1e-4,1]. The behaviour of the first correction is again explained by numerical errors.

In the right plot of Figure 8.10, we turn to an interesting question. Theorem 8.4 shows that observables are primarily transported along the classical flow with an error of $O(\varepsilon^2)$. Combining this result with the relation (1.4), one obtains the following result for the approximation of expectation-values in terms of the Wigner-function

$$\left| \langle \psi(t) | \mathrm{op}^{\varepsilon}(a) \psi(t) \rangle_{L^2(\mathbb{R}^d)} - \int_{\mathbb{R}^{2d}} \left(\mathcal{W}^{\varepsilon}(\psi(t)) \circ \kappa^{(s,t)} \right) (q,p) a(q,p) \, dq \, dp \right| \leq C\varepsilon^2,$$

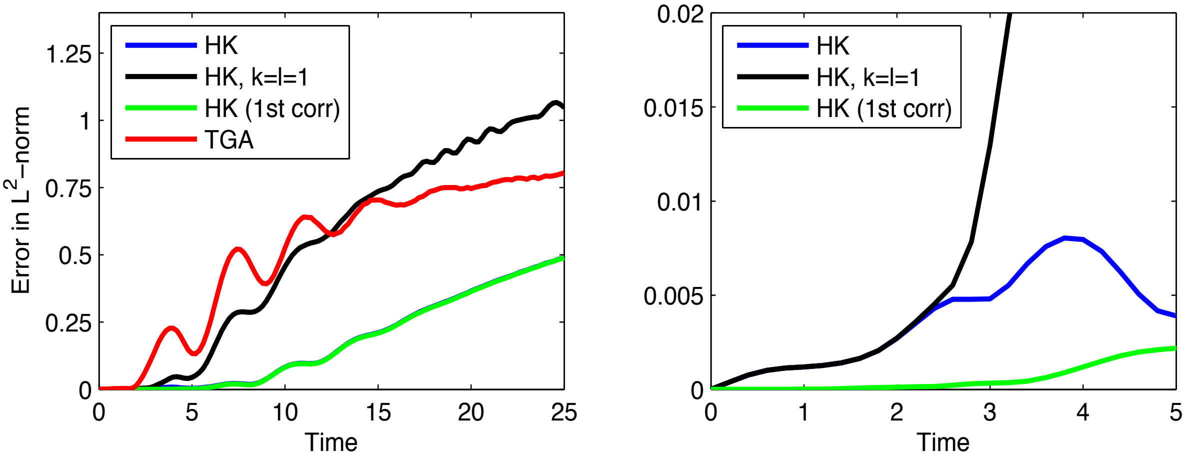

Figure 8.9: L^2-error of the IVRs for the quartic oscillator and $\varepsilon = 0.01$.

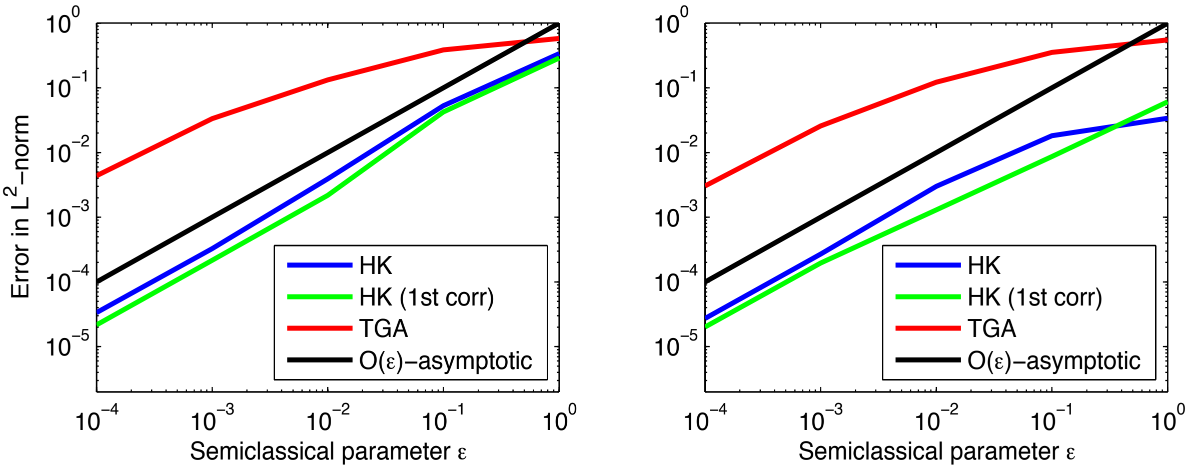

Figure 8.10: Asymptotic behaviour of the L^2-error for the quartic oscillator for $t = 5$.

where $\psi(t)$ is the solution of (1.8) and $a \in S[0; 2d]$ is subquadratic. One might wonder, if such a bound also holds for the approximation of expectation values by IVRs. As it is hard to prove the converse by analytic computations, we try to answer this question numerically.

The operator, whose expectation value we investigate is the simplest one possible, namely $\mathrm{op}^\varepsilon(1) = \mathrm{id}$. The obvious advantages of this choice lie in the fact that the exact expectation value is $\|\psi(t)\| = 1$ and thus known for all times and that the expectation value is independent of the quantization one chooses. Now the right plot in Figure 8.10 shows that the errors of the norms of the IVR-solutions behave like ε for $\varepsilon \to 0$. As this behaviour is shown even for small times one can rule out numerical problems and has to conclude that the bound in Proposition 8.5 is strict.

Part IV

Appendix

9 Summary of notation

We summarise the non-standard notation used in the dissertation and hint to its first appearance.

Spaces and sets

Notation	Denoted object	Defined in	Page
$S^\rho[\mathbf{m};\mathbf{d}], S[\mathbf{m};\mathbf{d}]$	Symbol-spaces	Definition 1.1	17
$\mathcal{C}, \mathcal{C}_{\text{const}}$	Accessible matrices for the FIOs	Definition 4.6	52

Transformations

Notation	Denoted object	Defined in	Page
$\mathcal{F}^\varepsilon$	Fourier transform	Equation (0.11)	10
$\mathcal{W}^\varepsilon$	Wigner transform	Equation (1.3)	16
$T^\varepsilon[\Theta]\,, T^\varepsilon_{\text{inv}}[\Theta]$	FBI-transform	Definition 4.2	45
$\mathcal{B}^\varepsilon$	Bargmann transform	Equation (4.5)	49
$\mathcal{H}^\varepsilon$	Husimi transform	Equation (4.7)	50

Operators

Notation	Denoted object	Defined in	Page
$\text{op}^\varepsilon(h)$	Weyl-quantization of h	Definition 1.2	17
$\mathcal{I}^\varepsilon_{\text{AW}}(\kappa; u; \Theta^x, \Theta^y)$	Anti-Wick Fourier Integral Operator	Definition 4.4	50
$\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$	Fourier Integral Operator	Definition 4.8	52
$\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$	Fourier Integral Operator	Definition 5.1	74
$D[\varepsilon]$	Dilation operator	Lemma 4.14	59

Special quantities

Notation	Denoted object	Defined in	Page
Φ^κ	Phase function of $\mathcal{I}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$	Equation (4.11)	52
Ψ^κ	Phase function of $\mathcal{R}^\varepsilon(\kappa; u; \Theta^x, \Theta^y)$	Equation (5.1)	73
$Z^\kappa, \overline{Z}^\kappa$	Complexifications of κ	Equation (7.20)	106
$\partial_z, \text{div}_z\,(f)$	Complex combinations of ∂_q and ∂_p	Equation (7.2)	98
F^κ	Jacobian of κ	Definition 2.1	28
$W(q,p)$	Matrix related to $\nabla_{(q,p)}\Phi^\kappa$	Equation (7.14)	103
$\mathcal{Z}(q,p)$	Matrix related to $\nabla_z\Phi^\kappa$	Equation (7.3)	98
c_κ, C_κ	Lipschitz-constants of κ	Proposition 2.3	28
$\Lambda(\Theta)$	Canonical transformation	Theorem 4.11	55

10 Omitted proofs

We collect some proofs which were omitted in the text due to their technicality.

10.1 The decay of the oscillatory integrals

We prove the decay properties of various operators used in this work. The following lemma concerns the differential operators used in the Definitions of PDOs and FIOs.

10.1 Lemma. *Let $w \in \mathcal{S}(\mathbb{R}^d)$.*

1. *Let*
$$L_{x'} := \frac{1 + i\varepsilon\xi \cdot \nabla_{x'}}{1 + |\xi|^2}.$$
There are constants $M_k^{(x')}[\varepsilon]$ such that
$$\left| \left(L_{x'}^\dagger \right)^k w(x) \right| \leq \frac{M_k^{(x')}[\varepsilon]}{\left(1 + |\xi|^2\right)^{k/2}} \sum_{\alpha \leq k} \left| \partial_{x'}^\alpha w(x) \right|. \tag{10.1}$$

2. *Let*
$$L_y := \frac{1 - i\varepsilon \left(-p + i\Theta^y(y-q)\right) \cdot \nabla_y}{1 + \left|-p + i\Theta^y(y-q)\right|^2}.$$
There are constants $M_k^{(y)}[\varepsilon, \Theta^y]$ such that
$$\left| \left(L_y^\dagger \right)^k w(x) \right| \leq \frac{M_k^{(y)}[\varepsilon, \Theta^y]}{\left(1 + \left|-p + i\Theta^y(y-q)\right|^2\right)^{k/2}} \sum_{\alpha \leq k} \left| \partial_y^\alpha w(x) \right|. \tag{10.2}$$

Proof.

1. By an application of the multinomial theorem we have
$$\left(L_{x'}^\dagger\right)^k = \left(\frac{1 - i\varepsilon\xi \cdot \nabla_{x'}}{1 + |\xi|^2}\right)^k = \langle\xi\rangle^{-2k} \sum_{k_1 + \ldots + k_{d+1} = k} \binom{n}{k_1, \ldots, k_{d+1}} (-i\varepsilon)^{k - k_{d+1}} \prod_{j=1}^d \left(\xi_j \partial_{x'_j}\right)^{k_j}.$$
Thus (10.1) follows from
$$\left\| \langle\xi\rangle^{-k} \prod_{j=1}^d \xi_j^{k_j} \right\|_{L^\infty(\mathbb{R}^d)} < \infty.$$

2. We set $f(y,q,p) := -p + i\Theta^y(y-q)$. By definition, we have

$$
\begin{aligned}
L_y^\dagger &= \frac{1 + i\varepsilon\left(-p + i\Theta^y(y-q)\right)\cdot\nabla_y}{1 + \left|-p + i\Theta^y(y-q)\right|^2} + \nabla_y \cdot \frac{i\varepsilon\left(-p + i\Theta^y(y-q)\right)}{1 + \left|-p + i\Theta^y(y-q)\right|^2} \\
&= \frac{1 + i\varepsilon f(y,q,p)\cdot\nabla_y}{1 + |f(y,q,p)|^2} + \nabla_y \cdot \frac{i\varepsilon f(y,q,p)}{1 + |f(y,q,p)|^2}.
\end{aligned} \tag{10.3}
$$

We show inductively that $\left(L_y^\dagger\right)^k$ is given by

$$
\left(L_y^\dagger\right)^k = \sum_{|\beta|\le k} g_\beta(y,q,p)\partial_y^\beta,
$$

where the functions g_β are sums of terms of the form

$$
C[\varepsilon, \Theta^x, \Theta^y] \frac{f(y,q,p)^\alpha \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^N}
$$

with $M, N \in \mathbb{N}$, $\alpha \in \mathbb{N}^d$, $|\alpha| \le k$, $|\alpha| \le N$ and $\alpha_{(j)} \in \mathbb{N}^d$ with $\left|\alpha_{(j)}\right| = 1$. As

$$
\left\| f_j(y,q,p) \left\langle f(y,q,p) \right\rangle^{-1} \right\|_{L^\infty(\mathbb{R}^{3d})} < \infty,
$$

this is enough to show the result.

For $k = 0$ the assertion is clear. For the induction step, we have $\partial_y^\gamma f(y,q,p) = 0$ for $|\gamma| \ge 2$ and thus

$$
\begin{aligned}
&\partial_{y_k} \frac{f(y,q,p)^\alpha \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^N} \\
&= \frac{\left(1 + |f(y,q,p)|^2\right)^N \sum_{l=1}^d f(y,q,p)^{\alpha - e_l} \partial_{y_k} f_l(x) \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^{2N}} \\
&\quad - \frac{\left[f(y,q,p)^\alpha \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)\right] \left(1 + |f(y,q,p)|^2\right)^{N-1} \sum_{l=1}^d 2 f_l(y,q,p) \partial_{y_k} f_l(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^{2N}} \\
&= \frac{\sum_{l=1}^d f(y,q,p)^{\alpha - e_l} \partial_{y_k} f_l(x) \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^N} \\
&\quad - \frac{\left[f(y,q,p)^\alpha \prod_{j=1}^M \partial_y^{\alpha_{(j)}} f(y,q,p)\right] \sum_{l=1}^d 2 f_l(y,q,p) \partial_{y_k} f_l(y,q,p)}{\left(1 + |f(y,q,p)|^2\right)^{N+1}}
\end{aligned}
$$

and the induction hypothesis on α and N combined with (10.3) yields the result.

□

The next lemma concerns the operators used in the proof of Theorems 4.11 and 5.4.

10.2 Lemma. *Let $w \in \mathcal{S}(\mathbb{R}^d)$.*

1. *Let $\varepsilon = 1$. There are constants $M_{k,l}^{(y,\xi)}$ such that*

$$\left|\partial_\xi^\gamma \left(L_y^\dagger\right)^k w\right| \leq \frac{M_{k,l}^{(y,\xi)}}{\left(1+|\xi|^2\right)^{k/2}} \sum_{\alpha\leq k,\beta\leq l} \left|\partial_y^\alpha \partial_\xi^\beta w\right|. \tag{10.4}$$

   for all $|\gamma| \leq l$.

2. *Let $\varepsilon = 1$ and $\Theta^x \in \mathcal{C}_{\text{const}}$. Furthermore let*

$$L_w = \frac{1 - i\varepsilon\,(\Theta)^{-1}\,\overline{f(w)}\cdot\nabla_w}{1+\left|(\Theta)^{-1/2} f(w)\right|^2},$$

   with

$$f(w) = C + i\Theta w, \quad C \in \mathbb{R}^d.$$

   There are Θ-independent constants $M_k^{(w)}$ such that

$$\left|\left(L_w^\dagger\right)^k u\right| \leq \frac{M_k^{(w)}}{\left(1+\left|(\Theta)^{-1/2} f(w)\right|^2\right)^{k/2}} \sum_{|\alpha|\leq k} \left|\left((\Theta)^{-1/2}\nabla_w\right)^\alpha u\right|,$$

Proof.

1. Recalling the proof of Lemma 10.1, it is enough to compute

$$\begin{aligned}\partial_{\xi_m}\left(\langle\xi\rangle^{-2k}\prod_{j=1}^d \xi_j^{k_j} w\right) &= \left(\langle\xi\rangle^{-2k}\prod_{j=1}^d \xi_j^{k_j}\right)(\partial_{\xi_m} w)\\ &+ \left((-2k)\,\langle\xi\rangle^{-2k-1}\,\xi_m \prod_{j=1}^d \xi_j^{k_j} + \langle\xi\rangle^{-2k}\,k_m \prod_{j=1}^d \xi_j^{k_j-\delta_{jm}}\right) w\end{aligned}$$

   to show the result, where δ_{jm} denotes the Kronecker symbol.

2. The decay for this type of operator was already shown in Lemma 10.1. The only thing left is to show the independence of the constants of Θ. As Θ and C are real, we can introduce the new variable $w' = \Theta^{\frac{1}{2}} w$, for which we have

$$\nabla_{w'} u(w(w')) = \nabla_w g(w(w'))\nabla_{w'} w(w') = \Theta^{-\frac{1}{2}}(\nabla_w g)(w(w')).$$

   Thus

$$L_w u(w) = \frac{1 - i\left[\Theta^{-\frac{1}{2}}C - iw'\right]\cdot\nabla_{w'}}{1+\left|\Theta^{-\frac{1}{2}}C + iw'\right|^2} u(w'(w)) =: L_{w'} u(w')$$

and the result follows from the arguments in Lemma 10.1.

□

10.2 On the sets $\mathcal{C}$ and $\mathcal{C}_{\text{const}}$

In this section, we present some results on the matrices used in the definition of our operators. For convenience of the reader, we recall the definition of the sets $\mathcal{C}$ and $\mathcal{C}_{\text{const}}$.

10.3 Definition (Accessible width-matrices)**.** *We define the set*

$$\mathcal{C} := \left\{ \Theta \in C^\infty \left(\mathbb{R}^{2d}, \mathbb{C}^{d\times d} \right) \cap S[0;2d] \middle| \Theta^\dagger = \Theta, \exists \Theta_0 \in \mathcal{C}_{\text{const}}, \Re\Theta - \Theta_0 \geq 0 \right\},$$

where

$$\mathcal{C}_{\text{const}} := \left\{ \Theta \in \mathbb{R}^{d\times d} \middle| \Theta^\dagger = \Theta, \Theta > 0 \right\}.$$

The elements of $\mathcal{C}_{\text{const}}$ are a special case of positive definite matrices.

10.4 Definition (Positive definite matrix)**.** *A matrix $\Theta \in \mathbb{C}^{d\times d}$ is called* ***positive definite****, if $\Re \langle z, \Theta z \rangle > 0 \; \forall z \in \mathbb{C}^d, z \neq 0$.*

Contrary to the situation of hermitian matrices, the property that $\sigma(A)$ is contained in the open right half-plane is only a necessary condition for a matrix A to be positive definite, but not a sufficient one. Consider the example

$$A = \begin{pmatrix} -1 & 2i \\ 2i & 3 \end{pmatrix}.$$

A has degenerate eigenvalue 1, eigenvector $(i,1)^\dagger$ and generalised eigenvector $(1,0)$, but is not positive definite as

$$\begin{pmatrix} 1 & 0 \end{pmatrix} A \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -1.$$

We collect some properties of positive definite matrices.

10.5 Lemma.

1. *$\Theta \in \mathbb{C}^{d\times d}$ is positive definite if and only if its hermitian part $(\Theta + \Theta^*)/2$ is positive in the sense of quadratic forms on $\mathbb{R}^d$.*
2. *A positive definite matrix is invertible with positive definite inverse. Moreover, the adjoint A^*, the transpose $A^\dagger$ and the complex conjugate $\overline{A}$ of a positive definite matrix A are positive definite as well.*
3. *A positive definite matrix Θ admits a unique positive definite square root, which is analytic in its argument Θ. If A is symmetric, i.e. $A^\dagger = A$, this square-root is symmetric as well.*

Proof.

1. Let $z \in \mathbb{C}^d$. We have

$$2\Re \langle z, \Theta z \rangle = \langle z, \Theta z \rangle + \overline{\langle z, \Theta z \rangle} = \langle z, \Theta z \rangle + \langle z, \Theta^* z \rangle = 2 \langle z, (\Re\Theta) z \rangle.$$

If $z = x + iy$ with $x, y \in \mathbb{R}^d$, we have $\langle z, \Re\Theta z \rangle = \langle x, \Re\Theta x \rangle + \langle y, \Re\Theta y \rangle$, hence the equivalence to positivity on $\mathbb{R}^d$.

2. A positive definite matrix is injective:

$$Ax = 0 \Rightarrow \Re \langle x, Ax \rangle = 0 \Rightarrow x = 0$$

and thus invertible. For its inverse we have

$$\Re \left\langle z, \Theta^{-1} z \right\rangle = \Re \left\langle \Theta \left(\Theta^{-1} z \right), \left(\Theta^{-1} z \right) \right\rangle > 0.$$

The other statements follow directly from $\Re(A^*) = \Re A$, $\langle x, \overline{A} x \rangle = \langle x, Ax \rangle$ for $x \in \mathbb{R}^d$ and $\overline{\Re(A)} = \Re(A^\dagger) = \Re(\overline{A})$.

3. Mirroring the ideas of [Kat66] V.§3.11, we define a matrix $M^{-1/2}$ by the Dunford-Taylor integral (see [Kat66] I.§5.6)

$$M^{-1/2} = \frac{1}{2\pi i} \int_\Gamma z^{-1/2} (M - z)^{-1} \, dz, \tag{10.5}$$

where the integration path is a closed contour in the half-plane $\{z | \Re z > 0\}$ making a turn around each eigenvalue in the positive direction and the value of $z^{1/2}$ is chosen so that it is positive for real positive z. As a consequence, $M^{-1/2}$ is an holomorphic function of M^{-1}.

$M^{-1/2}$ is a square root of M^{-1}: Let Γ_1, Γ_2 be two closed contours as described, with Γ_1 lying completely in the interior of Γ_2. Using the resolvent identity, we have

$$\begin{aligned}
\left(M^{-1/2} \right)^2 &= \frac{1}{2\pi i} \int_{\Gamma_1} \int_{\Gamma_2} z_1^{-1/2} z_2^{-1/2} (z_1 - M)^{-1} (z_2 - M)^{-1} \, dz_1 \, dz_2 \\
&= \frac{1}{2\pi i} \int_{\Gamma_1} \int_{\Gamma_2} z_1^{-1/2} z_2^{-1/2} \frac{(z_1 - M)^{-1} - (z_2 - M)^{-1}}{z_2 - z_1} \, dz_1 \, dz_2 \\
&= \frac{1}{2\pi i} \int_{\Gamma_1} z_1^{-1/2} (z_1 - M)^{-1} \left[\frac{1}{2\pi i} \int_{\Gamma_2} \frac{z_2^{1/2}}{z_2 - z_1} \, dz_2 \right] dz_1 \\
&\quad - \frac{1}{2\pi i} \int_{\Gamma_2} z_2^{-1/2} (z_2 - M)^{-1} \left[\frac{1}{2\pi i} \int_{\Gamma_1} \frac{z_1^{-1/2}}{z_2 - z_1} \, dz_1 \right] dz_2 \\
&= \frac{1}{2\pi i} \int_{\Gamma_1} z_1^{-1} (M - z_1)^{-1} \, dz_1 = M^{-1}.
\end{aligned}$$

To show that this square root is positive definite, we deform the integration contour such that it runs from $-R$ to 0 along the edge of the negative x-axis, makes a turn around the origin in positive direction, runs back to $-R$ along the upper edge of the negative x-axis and runs along $Re^{-i\lambda}, \lambda \in]-\pi, \pi[$ to close the circle. Here, R is chosen large enough such that it encloses the spectrum of M. Taking the limit $R \to \infty$, the integral along $Re^{-i\lambda}, \lambda \in]-\pi, \pi[$ tends to zero and we obtain the expression

$$M^{-1/2} = \frac{1}{\pi} \int_0^\infty R^{-1/2} (M + \lambda)^{-1} \, dR$$

for the square-root. Now $(M + R)^{-1}$ is positive definite and hence we get the positivity of the square root.

As
$$M = \frac{1}{2\pi i}\int_\Gamma z^{-1}(M^{-1}-z)^{-1}\,dz, \tag{10.6}$$
we see that $M^{1/2}$ is an analytic function of M, which is positive because of Assertion 2.

The uniqueness of the positive square-root follows from matrix theory, see [JOR01], Theorem 5. Finally, we show that the square-root of a symmetric matrix A is symmetric. Then
$$A^{1/2}A^{1/2} = A = A^\dagger = \left(A^{1/2}\right)^\dagger\left(A^{1/2}\right)^\dagger$$
and thus $\left(A^{1/2}\right)^\dagger = A^{1/2}$ by the uniqueness of the positive definite square root. Alternatively, the symmetry can be seen directly from (10.5).

□

For the elements of $\mathcal{C}$ we have the following Lemma:

10.6 Lemma. *Let $\Theta \in \mathcal{C}$. Then $\Theta^{-1} \in \mathcal{C}$ and there is a unique square-root $\Theta^{\frac{1}{2}} \in \mathcal{C}$.*

Proof. We treat the inverse first. As $\Theta \in \mathcal{C}$, there is $c_\Theta > 0$ such that
$$\Re\left\langle \Theta(q,p)z|z\right\rangle \geq c_\Theta\,|z|^2 \qquad \forall z \in \mathbb{C}^d, (q,p)\in\mathbb{R}^{2d}.$$
Hence
$$\begin{aligned}\Re\left\langle z, \Theta^{-1}(q,p)z\right\rangle &= \Re\left\langle \Theta(q,p)\left(\Theta^{-1}(q,p)z\right), \left(\Theta^{-1}(q,p)z\right)\right\rangle \\ &\geq c_\Theta\left|\Theta^{-1}(q,p)z\right|^2 \geq \frac{c_\Theta\,|z|^2}{\|\Theta(q,p)\|^2_{L^\infty(\mathbb{R}^{2d})}} \qquad \forall z\in\mathbb{R}^d\end{aligned}$$
and we have established the bound away from zero by the matrix
$$\Theta_0 := \frac{c_\Theta \mathrm{id}}{\|\Theta(q,p)\|^2_{L^\infty(\mathbb{R}^{2d})}}.$$
We turn to the symbol class of Θ^{-1}, i.e. the smoothness and the boundedness of Θ^{-1} with respect to (q,p), which can be seen from the Dunford-Taylor integral (10.6).

In Lemma 10.5 we have already established the existence, uniqueness and smoothness of $\Theta^{\frac{1}{2}}(q,p)$. As the smoothness of the square root and the compactness of
$$\left\{\Theta\in\mathbb{C}^{d\times d}\middle|\Theta=\Theta^\dagger, \Theta_0 \leq \Theta \leq \|\Theta\|_{L^\infty(\mathbb{R}^{2d})}\right\}$$
an upper bound for the square root, it remains to show a uniform bound from below, which follows from
$$\begin{aligned}\Re\left\langle z, \Theta^{\frac{1}{2}}(q,p)z\right\rangle &= \Re\left\langle\left(\Theta^{-\frac{1}{2}}(q,p)z\right), \Theta(q,p)\left(\Theta^{-\frac{1}{2}}(q,p)z\right)\right\rangle \\ &\geq c_\Theta\left|\Theta^{-\frac{1}{2}}(q,p)z\right|^2 \geq \frac{c_\Theta\,|z|^2}{\left\|\Theta^{\frac{1}{2}}(q,p)\right\|^2_{L^\infty(\mathbb{R}^{2d})}} \qquad \forall z\in\mathbb{R}^d.\end{aligned}$$

□

10.3 On the matrices $W(q,p)$ and $\mathcal{Z}(q,p)$

We discuss the matrices $W(q,p)$ and $\mathcal{Z}(q,p)$.

10.7 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$ and $\Theta^x, \Theta^y \in \mathcal{C}$. The matrix*

$$W(q,p) := \left(\begin{array}{c|c} (F^\kappa)^\dagger (q,p) \begin{pmatrix} -i\Theta^x(q,p) \\ \mathrm{id} \end{pmatrix} & \begin{matrix} -i\Theta^y(q,p) \\ -\mathrm{id} \end{matrix} \end{array} \right)$$

is invertible with $\left(W^\kappa[\Theta^x,\Theta^y]\right)^{-1}(q,p) \in S[0;2d]$. In the Ehrenfest case $T(\varepsilon) = C_T \log\left(\varepsilon^{-1}\right)$, we have

$$\left\|\partial^\alpha_{(q,p)} W^\kappa[\Theta^x,\Theta^y]\right\|_{L^\infty_{(q,p)}} \leq C_\rho \varepsilon^{-\rho} \quad \text{and} \quad \left\|\partial^\alpha_{(q,p)} \left(W^\kappa[\Theta^x,\Theta^y]\right)^{-1}\right\|_{L^\infty_{(q,p)}} \leq C_\rho \varepsilon^{-\rho}$$

for all $\alpha \in \mathbb{N}^d$, where ρ can be made arbitrary small if C_T chosen small enough.

Proof. For better readability, we drop the arguments of W, F^κ, Θ^x and Θ^y. We have

$$\begin{aligned}
&W \begin{pmatrix} (\Re\Theta^x)^{-1} & \\ & (\Re\Theta^y)^{-1} \end{pmatrix} W^* \\
&= \left(\begin{array}{c|c} (F^\kappa)^\dagger \begin{pmatrix} -i\Theta^x \\ \mathrm{id} \end{pmatrix} & \begin{matrix} -i\Theta^y \\ -\mathrm{id} \end{matrix} \end{array} \right) \begin{pmatrix} (\Re\Theta^x)^{-1} & \\ & (\Re\Theta^y)^{-1} \end{pmatrix} \left(\begin{array}{c|c} (F^\kappa)^\dagger \begin{pmatrix} -i\Theta^x \\ \mathrm{id} \end{pmatrix} & \begin{matrix} -i\Theta^y \\ -\mathrm{id} \end{matrix} \end{array} \right)^* \\
&= (F^\kappa)^\dagger \begin{pmatrix} \Im\Theta^x (\Re\Theta^x)^{-1} - i\,\mathrm{id} \\ (\Re\Theta^x)^{-1} \end{pmatrix} \begin{pmatrix} i\overline{\Theta^x} & \mathrm{id} \end{pmatrix} F^\kappa + \begin{pmatrix} \Im\Theta^y (\Re\Theta^y)^{-1} - i\,\mathrm{id} \\ -(\Re\Theta^y)^{-1} \end{pmatrix} \begin{pmatrix} i\overline{\Theta^y} & -\mathrm{id} \end{pmatrix} \\
&= (F^\kappa)^\dagger \begin{pmatrix} i\Im\Theta^x + \Im\Theta^x (\Re\Theta^x)^{-1} \Im\Theta^x + \overline{\Theta^x} - i\,\mathrm{id} & \Im\Theta^x (\Re\Theta^x)^{-1} - i\,\mathrm{id} \\ (\Re\Theta^x)^{-1} \Im\Theta^x + i\,\mathrm{id} & (\Re\Theta^x)^{-1} \end{pmatrix} F^\kappa \\
&\quad + \begin{pmatrix} i\Im\Theta^y + \Im\Theta^y (\Re\Theta^y)^{-1} \Im\Theta^y + \overline{\Theta^y} - i\,\mathrm{id} & -\Im\Theta^y (\Re\Theta^y)^{-1} + i\,\mathrm{id} \\ -(\Re\Theta^y)^{-1} \Im\Theta^y - i\,\mathrm{id} & (\Re\Theta^y)^{-1} \end{pmatrix} \\
&= (F^\kappa)^\dagger (\Lambda(\Theta^x))^\dagger \Lambda(\Theta^x) F - i (F^\kappa)^\dagger J F^\kappa + \left(\Lambda\left(\overline{\Theta^y}\right)\right)^\dagger \Lambda\left(\overline{\Theta^y}\right) + iJ \\
&= (\Lambda(\Theta^x)F^\kappa)^\dagger (\Lambda(\Theta^x)F^\kappa) + \left(\Lambda\left(\overline{\Theta^y}\right)\right)^\dagger \Lambda\left(\overline{\Theta^y}\right)
\end{aligned} \tag{10.7}$$

where we have introduced the symplectic matrix

$$\Lambda(\Theta) = \begin{pmatrix} (\Re\Theta)^{\frac{1}{2}} & 0 \\ (\Re\Theta)^{-\frac{1}{2}} \Im\Theta & (\Re\Theta)^{-\frac{1}{2}} \end{pmatrix}$$

which fulfills

$$\Lambda(\Theta)^\dagger \Lambda(\Theta) = \begin{pmatrix} \Re\Theta + \Im\Theta (\Re\Theta)^{-1} \Im\Theta & \Im\Theta (\Re\Theta)^{-1} \\ (\Re\Theta)^{-1} \Im\Theta & (\Re\Theta)^{-1}. \end{pmatrix}$$

The matrix in (10.7) is invertible as the sum of two real symmetric positive definite matrices, we get the invertibility of

$$W \begin{pmatrix} (\Re\Theta^x)^{-1} & \\ & (\Re\Theta^y)^{-1} \end{pmatrix} W^*$$

and with it the invertibility of $W(q,p)$.

We turn to the symbol class of $W(q,p)$. As κ is of class $\mathcal{B}$, we have $W(q,p) \in S[0;2d]$ so it remains to show that the inverse of the matrix in (10.7) is $S[0;2d]$. As the inverse of a matrix A max be expressed as

$$A^{-1} = \frac{1}{\det A} \begin{pmatrix} A_{11} & -A_{21} & \dots & (-1)^{d+1}A_{d1} \\ -A_{12} & A_{22} & \dots & (-1)^{d+2}A_{d2} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{d+1}A_{1d} & (-1)^{d+2}A_{2d} & \dots & A_{dd} \end{pmatrix}, \tag{10.8}$$

where the A_{kl} denote the minors of the matrix A. Hence it is enough to prove a bound from below for the determinant. By the concavity inequality

$$[\det(A+B)]^{1/d} \geq (\det A)^{1/d} + (\det B)^{1/d}$$

for real symmetric positive matrices A and B we have

$$|\det W(q,p)|^2\,(\det \Re\Theta^x)^{-1}(\det \Re\Theta^y)^{-1} \geq |\det(\Lambda(\Theta^y))|^2 = 1$$

and hence

$$|\det W(q,p)| \geq (\det \Re\Theta^x)^{\frac{1}{2}}(\det \Re\Theta^y)^{\frac{1}{2}} \geq (\det \Theta_0^x)^{\frac{1}{2}}(\det \Theta_0^y)^{\frac{1}{2}},$$

where we used

$$\det(\Re\Theta^x) = \det(\Re\Theta^x - \Theta_0^x + \Theta_0^x) \geq \left[\det(\Re\Theta^x - \Theta_0^x)^{1/d} + \det(\Theta_0^x)^{1/d}\right]^d \geq \det(\Theta_0^x).$$

The bounds for the Ehrenfest case follow from Proposition 2.7 and the expression for $W^{-1}(q,p)$ by the formula of minors (10.8). □

10.8 Lemma. *Let κ be a canonical transformation of class $\mathcal{B}$ and $\Theta^x, \Theta^y \in \mathcal{C}$. The matrix*

$$\mathcal{Z}(q,p) := (i\,(\Theta^y)^{-1} \quad \mathrm{id})(F^\kappa(q,p))^\dagger(-i\Theta^x \quad \mathrm{id})^\dagger.$$

is invertible and its inverse $\mathcal{Z}^{-1}(q,p)$ is in the class $S[0;2d]$. In the Ehrenfest case $T(\varepsilon) = C_T \log(\varepsilon^{-1})$, we have

$$\left\|\partial^\alpha_{(q,p)}\mathcal{Z}\right\|_{L^\infty_{(q,p)}} \leq C_\rho\varepsilon^{-\rho} \quad \textit{and} \quad \left\|\partial^\alpha_{(q,p)}\mathcal{Z}^{-1}\right\|_{L^\infty_{(q,p)}} \leq C_\rho\varepsilon^{-\rho} \tag{10.9}$$

for all $\alpha \in \mathbb{N}^d$, where ρ becomes arbitrary small for $C_T \to 0$.

Proof. The argumentation is analogue to the one in Lemma 10.7, as

$$\begin{aligned}&\mathcal{Z}(q,p)\,(\Re\Theta^x)^{-1}\,\mathcal{Z}(q,p)^* \\ &= 2\Re\,(\Theta^y)^{-1} + \left(\Lambda\,(\Theta^x)\,F^\kappa(q,p)\begin{pmatrix} i\,(\Theta^y)^{-1} \\ -\mathrm{id}\end{pmatrix}\right)^*\left(\Lambda\,(\Theta^x)\,F^\kappa(q,p)\begin{pmatrix} i\,(\Theta^y)^{-1} \\ -\mathrm{id}\end{pmatrix}\right)\end{aligned}$$

and thus

$$|\det(\mathcal{Z}(q,p))| \geq \det\left(2\Re\,(\Theta^y(q,p))^{-1/2}\right)\det(\Re\Theta^x(q,p))^{\frac{1}{2}}.$$

□

10.4 Taylor expansion in complex variables

We justify the Taylor expansion in the complex "variables" a and $\overline{a}$, which is used in the proof of Propositions 7.3 and 7.5.

10.9 Lemma. *Let $f : \mathbb{N}^d \to \mathbb{C}$. We have*

$$\sum_{|\alpha|=N+1} f(\alpha) = \frac{1}{N+1} \sum_{|\alpha|=N} \sum_{j=1}^{d} (\alpha_j + 1) f(\alpha + e_j).$$

Proof. For $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$, we set

$$\alpha \wedge j := (\alpha_1, \ldots, \alpha_{j-1}, \alpha_{j+1}, \ldots, \alpha_d).$$

The result follows by induction, as

$$\begin{aligned}
\sum_{|\alpha|=N+1} f(\alpha) &= \frac{1}{N+1} \sum_{|\alpha|=N+1} f(\alpha) \sum_{j=1}^{d} \alpha_j = \frac{1}{N+1} \sum_{j=1}^{d} \sum_{\alpha_j=0}^{N+1} \sum_{\substack{|\alpha\wedge j| \\ =N+1-\alpha_j}} \alpha_j f(\alpha) \\
&= \frac{1}{N+1} \sum_{j=1}^{d} \sum_{\alpha_j=0}^{N} \sum_{\substack{|\alpha\wedge j| \\ =N-\alpha_j}} (\alpha_j + 1) f(\alpha + e_j) \\
&= \frac{1}{N+1} \sum_{|\alpha|=N} \sum_{j=1}^{d} (\alpha_j + 1) f(\alpha + e_j).
\end{aligned}$$

□

10.10 Lemma. *Let $h \in S[+\infty; 2d]$. We have*

$$\begin{aligned}
h(x, \xi) = &\sum_{|\alpha+\beta|\leq N} \frac{1}{\alpha!\beta!} \left(\left(\partial_a^\alpha \partial_{\overline{a}}^\beta h \right) \circ \kappa \right) (q, p) \left(a - Z^\kappa(q, p) \right)^\alpha \left(\overline{a} - \overline{Z}^\kappa(q, p) \right)^\beta \\
&+ \sum_{|\alpha+\beta|=N+1} \left(a - Z^\kappa(q, p) \right)^\alpha \left(\overline{a} - \overline{Z}^\kappa(q, p) \right)^\beta R_{\alpha,\beta}(a, \overline{a}, q, p),
\end{aligned}$$

where

$$\begin{aligned}
&R_{\alpha,\beta}(a, \overline{a}, q, p) \\
&= \frac{|\alpha+\beta|}{\alpha!\beta!} \int_0^1 \sigma^{|\alpha+\beta|-1} \left(\partial_a^\alpha \partial_{\overline{a}}^\beta h \right) \left(x + \sigma \left(X^\kappa(q, p) - x \right), \xi + \sigma \left(\Xi^\kappa(q, p) - \xi \right) \right) d\sigma.
\end{aligned}$$

Proof. The Taylor expansion of

$$g(\tau) = h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa) \right)$$

around $\tau = 0$ to order N evaluated at $\tau = 1$ reads

$$g(\tau) = \sum_{k \le N} \frac{1}{k!} \left[\frac{d^k}{d\tau^k} h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right) \right]_{\tau=0} + \int_0^1 \frac{1}{N!} \left[\frac{d^{N+1}}{d\tau^{N+1}} h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right) \right]_{\tau=\sigma} d\sigma.$$

It is straightforward to check that

$$\begin{aligned} &\frac{d}{d\tau} h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right) \\ &= (\partial_a h)\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right)(a - Z^\kappa(q,p)) \\ &\quad + (\partial_{\overline{a}} h)\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right)(\overline{a} - \overline{Z}^\kappa(q,p)) \end{aligned}$$

and thus

$$\begin{aligned} &\left[\frac{d^k}{d\tau^k} h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right) \right]_{\tau=0} \\ &= \sum_{|\alpha+\beta|=k} \frac{k+1}{\alpha!\beta!} \left((\partial_a^\alpha \partial_{\overline{a}}^\beta h) \circ \kappa \right)(q,p)(a - Z^\kappa(q,p))^\alpha (\overline{a} - \overline{Z}^\kappa(q,p))^\beta \end{aligned}$$

by induction:

$$\begin{aligned} &\left[\frac{d^{k+1}}{d\tau^{k+1}} h\left(X^\kappa + \tau(x - X^\kappa), \Xi^\kappa + \tau(\xi - \Xi^\kappa)\right) \right]_{\tau=0} \\ &= \sum_{|\alpha+\beta|=k} \frac{k+1}{\alpha!\beta!} \left[\sum_{l_1=1}^{d} \left((\partial_a^{\alpha+e_{l_1}} \partial_{\overline{a}}^\beta h) \circ \kappa \right)(q,p)(a - Z^\kappa(q,p))^{\alpha+e_{l_1}} (\overline{a} - \overline{Z}^\kappa(q,p))^\beta \right. \\ &\qquad \left. + \sum_{l_2=1}^{d} \left((\partial_a^\alpha \partial_{\overline{a}}^{\beta+e_{l_2}} h) \circ \kappa \right)(q,p)(a - Z^\kappa(q,p))^\alpha (\overline{a} - \overline{Z}^\kappa(q,p))^{\beta+e_{l_2}} \right] \\ &= \sum_{|\alpha+\beta|=k+1} \frac{k+2}{\alpha!\beta!} \left((\partial_a^\alpha \partial_{\overline{a}}^\beta h) \circ \kappa \right)(q,p)(a - Z^\kappa(q,p))^\alpha (\overline{a} - \overline{Z}^\kappa(q,p))^\beta \end{aligned}$$

where we used Lemma 10.9. □

11 Some technical results

We collect some basic technical results used in the dissertation for convenience of the reader.

11.1 Faà di Bruno's formula

The generalisation of the chain rule to higher derivatives is known as Faà di Bruno's formula. The following version is taken from [Har06].

11.1 Proposition. *Let $f \in C^n(\mathbb{R}^d, \mathbb{C})$. We have*

$$\frac{\partial^n}{\partial x_1 \dots \partial x_n} f(y) = \sum_\pi f^{(|\pi|)}(y) \prod_{B \in \pi} \frac{\partial^{|B|} y}{\prod_{j \in B} \partial x_j}, \tag{11.1}$$

where π runs over all partitions of the set $\{1, \dots n\}$.

11.2 Symplectic matrices

We recall that a matrix $M \in \mathbb{R}^{2d \times 2d}$ is symplectic if and only if it fulfills

$$M^\dagger J M = J,$$

which is equivalent to

$$M^{-1} = -J M^\dagger J.$$

Hence the block decomposition

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

yields

$$\begin{aligned} AD^\dagger - BC^\dagger &= \mathrm{id} & BA^\dagger - AB^\dagger &= 0 \\ DA^\dagger - CB^\dagger &= \mathrm{id} & CD^\dagger - DC^\dagger &= 0 \end{aligned}$$

$$\begin{aligned} D^\dagger A - B^\dagger C &= \mathrm{id} & D^\dagger B - B^\dagger D &= 0 \\ A^\dagger D - C^\dagger B &= \mathrm{id} & A^\dagger C - C^\dagger A &= 0. \end{aligned}$$

Applying this to the symplectic matrix

$$F^\kappa(q,p) = \begin{pmatrix} X_q^\kappa(q,p)^\dagger & X_p^\kappa(q,p)^\dagger \\ \Xi_q^\kappa(q,p)^\dagger & \Xi_p^\kappa(q,p)^\dagger \end{pmatrix},$$

we have the identities

$$\begin{aligned}
X_q^\kappa(q,p)^\dagger \Xi_p^\kappa(q,p) - X_p^\kappa(q,p)^\dagger \Xi_q^\kappa(q,p) &= \mathrm{id} \\
\Xi_p^\kappa(q,p)^\dagger X_q^\kappa(q,p) - \Xi_q^\kappa(q,p)^\dagger X_p^\kappa(q,p) &= \mathrm{id} \\
X_p^\kappa(q,p)^\dagger X_q^\kappa(q,p) - X_q^\kappa(q,p)^\dagger X_p^\kappa(q,p) &= 0 \\
\Xi_q^\kappa(q,p)^\dagger \Xi_p^\kappa(q,p) - \Xi_p^\kappa(q,p)^\dagger \Xi_q^\kappa(q,p) &= 0
\end{aligned}$$

$$\begin{aligned}
\Xi_p^\kappa(q,p) X_q^\kappa(q,p)^\dagger - X_p^\kappa(q,p) \Xi_q^\kappa(q,p)^\dagger &= \mathrm{id} \\
X_q^\kappa(q,p) \Xi_p^\kappa(q,p)^\dagger - \Xi_q^\kappa(q,p) X_p^\kappa(q,p)^\dagger &= \mathrm{id} \\
\Xi_p^\kappa(q,p) X_p^\kappa(q,p)^\dagger - X_p^\kappa(q,p) \Xi_p^\kappa(q,p)^\dagger &= 0 \\
X_q^\kappa(q,p) \Xi_q^\kappa(q,p)^\dagger - \Xi_q^\kappa(q,p) X_q^\kappa(q,p)^\dagger &= 0.
\end{aligned}$$

11.3 Some results on coherent states

11.2 Lemma. *Let $M \in \mathbb{C}^{d\times d}$ be symmetric and positive definite. We have*

$$\frac{1}{(2\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon}\, dx = \det\left(M^{-1/2}\right), \tag{11.2}$$

where $M^{-1/2}$ is the unique positive definite square root of M^{-1}.

Proof. The Gaussian integral

$$\frac{1}{(2\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon}\, dx,$$

is analytic in M. For real positive definite matrices, it is well-known that its value is given by $(\det M)^{-1/2} = \det(M^{-1/2})$. Now the integral on the left-hand side of (11.2) is analytic in M and thus the assertion follows by analytic continuation and Lemma 10.5. □

11.3 Lemma (Fourier-transform of a coherent state)**.** *Let $M \in \mathbb{C}^{d\times d}$ be symmetric and positive definite. We have*

$$\begin{aligned}
&\frac{1}{(2\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} e^{-ik\cdot x/\varepsilon} \left[\tfrac{\det(\Re M)^{\frac14}}{(\pi\varepsilon)^{d/4}} e^{-M(x-x_0)^2/2\varepsilon + ik_0\cdot(x-x_0)/\varepsilon} \right] dx \\
&= \det\left(M^{-1/2}\right) \tfrac{\det(\Re M)^{\frac14}}{(\pi\varepsilon)^{d/4}} e^{-M^{-1}(k-k_0)^2/2\varepsilon - ik\cdot x_0/\varepsilon},
\end{aligned}$$

where $M^{-1/2}$ is the unique positive definite square root of M^{-1}. Note that

$$\left| \frac{\det(\Re M)^{1/4}}{\det M^{1/2}} \right| = \det\left(\Re(M^{-1})\right)^{1/4}.$$

Proof. We follow the strategy taken in Appendix A of [Fol89] and treat the case $x_0 = \xi_0 = 0$

first. We have

$$\nabla_k \left[\int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx \right] = \int_{\mathbb{R}^d} \frac{ix}{\varepsilon} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx$$

$$= -iM^{-1} \int_{\mathbb{R}^d} \frac{-Mx}{\varepsilon} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx = -iM^{-1} \int_{\mathbb{R}^d} \left[\nabla_x e^{-Mx^2/2\varepsilon} \right] e^{ik\cdot x/\varepsilon}\, dx$$

$$= iM^{-1} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon} \left[\nabla_x e^{ik\cdot x/\varepsilon} \right]\, dx = \frac{-M^{-1}k}{\varepsilon} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx$$

And hence

$$\nabla_k \left[e^{M^{-1}k^2/2\varepsilon} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx \right],$$

i.e.

$$(2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon + ik\cdot x/\varepsilon}\, dx = C[M] e^{-M^{-1}k^2/2\varepsilon},$$

where the contant $C[M]$ is deduced from $k = 0$:

$$C[M] = (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon}\, dx = \det \left(M^{-1/2} \right)$$

by Lemma 11.2. For the general case, we have

$$\int_{\mathbb{R}^d} e^{-ik\cdot x/\varepsilon} e^{-M(x-x_0)^2/2\varepsilon + ik_0\cdot(x-x_0)/\varepsilon}\, dx = \int_{\mathbb{R}^d} e^{-ik\cdot(x+x_0)/\varepsilon} e^{-Mx^2/2\varepsilon + ik_0\cdot x/\varepsilon}\, dx$$

$$= e^{-ikx_0/\varepsilon} \int_{\mathbb{R}^d} e^{-Mx^2/2\varepsilon + i(k_0-k)\cdot x/\varepsilon}\, dx = e^{-ikx_0/\varepsilon} e^{-M^{-1}(k-k_0)^2/2\varepsilon}\, dx.$$

It remains to show that

$$\left| \frac{\det \Re M}{\det M^2} \right| = \det \Re(M^{-1}).$$

Let $M = A + iB$ and $C = \Re(A+iB)^{-1}$. We have

$$2C = (A+iB)^{-1} + (A-iB)^{-1} \Leftrightarrow (A+iB)C(A-iB) = A$$

and thus

$$\left| \frac{\det \Re M}{\det M^2} \right| = \frac{\det(MCM^*)}{\det(MM^*)} = \det(C).$$

□

11.4 Lemma (Inner product of coherent states)**.**
Let $x_1, x_2, \xi_1, \xi_2 \in \mathbb{R}^d$, $\Theta_1, \Theta_2 \in \mathbb{C}^{d\times d}$ symmetric positive definite. We have

$$\left\langle g^{\varepsilon,\overline{\Theta_1}}_{(x_1,\xi_1)} \middle| g^{\varepsilon,\Theta_2}_{(x_2,\xi_2)} \right\rangle_{L^2(\mathbb{R}^d)} = \frac{(\det \Re\Theta_1 \det \Re\Theta_2)^{\frac{1}{4}}}{\det \left(\frac{1}{2} (\Theta_1 + \Theta_2)^{\frac{1}{2}} \right)}$$
$$\times \exp \left[-2\delta_\xi \cdot (\Theta_1 + \Theta_2)^{-1} \delta_\xi/\varepsilon - 2\Theta_1 \delta_x \cdot (\Theta_1 + \Theta_2)^{-1} \Theta_2 \delta_x/\varepsilon \right]$$
$$\times \exp \left[2i\delta_\xi \cdot (\Theta_1 + \Theta_2)^{-1} (\Theta_2 - \Theta_1)\delta_x/\varepsilon \right]$$
$$\times \exp \left[i(x_1 - x_2)\cdot(\xi_1 + \xi_2)/2\varepsilon \right],$$

where

$$\delta_\xi = \frac{\xi_1 - \xi_2}{2}, \qquad \delta_x = \frac{x_1 - x_2}{2}$$

and $(\Theta_1 + \Theta_2)^{\frac{1}{2}}$ *is the unique positive definite square root of* $\Theta_1 + \Theta_2$*. Moreover, if* $\Re\Theta_1, \Re\Theta_2 > \Theta_0 > 0$ *and* $\Re\left(\Theta_1^{-1}\right), \Re\left(\Theta_2^{-1}\right) > \Theta_0'$*, we have*

$$\left|\left\langle g^{\varepsilon,\overline{\Theta_1}}_{(x_1,\xi_1)} \middle| g^{\varepsilon,\Theta_2}_{(x_2,\xi_2)} \right\rangle_{L^2(\mathbb{R}^d)}\right|^2 \leq C[\Theta_1, \Theta_2, \Theta_0, \Theta_0'] e^{-\Theta_0(x_1-x_2)^2/4\varepsilon} e^{-\Theta_0'(\xi_1-\xi_2)^2/4\varepsilon},$$

where the constant $C[\Theta_1, \Theta_2, \Theta_0, \Theta_0']$ *is* ε*-independent.*

Proof. We define

$$\hat{x} = \frac{x_1 + x_2}{2}, \qquad \delta_x = \frac{x_1 - x_2}{2}, \qquad \hat{\xi} = \frac{\xi_1 + \xi_2}{2}, \qquad \delta_\xi = \frac{\xi_1 - \xi_2}{2} \qquad \text{and}$$
$$\delta_x^\Theta = (\Theta_1 + \Theta_2)^{-1}(\Theta_2 - \Theta_1)\delta_x$$

The inner product is given by the integral

$$\frac{(\det \Re\Theta_1 \det \Re\Theta_2)^{\frac{1}{4}}}{(\pi\varepsilon)^{\frac{d}{2}}} \int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\Omega(x,x_1,x_2,\xi_1,\xi_2)} dx,$$

where

$$\begin{aligned}\Omega(x, x_1, x_2, \xi_1, \xi_2) &= \xi_2 \cdot (x - x_2) - \xi_1 \cdot (x - x_1) \\ &\quad + i\Theta_1(x - x_1)^2/2 + i\Theta_2(x - x_2)^2/2\end{aligned}$$

By explicit algebraic manipulations, we have

$$\begin{aligned}\Omega &= 2\delta_\xi \cdot (\hat{x} - x) + 2\delta_x \cdot \hat{\xi} \\ &\quad + i(\Theta_1 + \Theta_2)(x - \hat{x})^2/2 + i(x - \hat{x}) \cdot (\Theta_2 - \Theta_1)\delta_x + i(\Theta_1 + \Theta_2)\delta_x^2/2 \\ &= 2\delta_\xi \cdot (\hat{x} - x) + 2\delta_x \cdot \hat{\xi} \\ &\quad + i(\Theta_1 + \Theta_2)(x - \hat{x})^2/2 + i(x - \hat{x}) \cdot (\Theta_1 + \Theta_2)\delta_x^\Theta \\ &\quad + i(\Theta_1 + \Theta_2)\left(\delta_x^\Theta\right)^2/2 - i(\Theta_1 + \Theta_2)\left(\delta_x^\Theta\right)^2/2 + i(\Theta_1 + \Theta_2)\delta_x^2/2 \\ &= -2\delta_\xi \cdot (x - \hat{x} + \delta_x^\Theta) + 2\delta_x \cdot \hat{\xi} + 2\delta_\xi \cdot \delta_x^\Theta \\ &\quad + i(\Theta_1 + \Theta_2)(x - \hat{x} + \delta_x^\Theta)^2/2 + i(\Theta_1 + \Theta_2)\delta_x^2/2 - i(\Theta_1 + \Theta_2)\left(\delta_x^\Theta\right)^2/2 \\ &= -2\delta_\xi \cdot (x - \hat{x} + \delta_x^\Theta) + 2\delta_x \cdot \hat{\xi} + 2\delta_\xi \cdot \delta_x^\Theta \\ &\quad + i(\Theta_1 + \Theta_2)(x - \hat{x} + \delta_x^\Theta)^2/2 + 2i\Theta_1\delta_x \cdot (\Theta_1 + \Theta_2)^{-1}\Theta_2\delta_x.\end{aligned}$$

Hence, the integral is the Fourier-Transform of a Gaussian evaluated at $k = 0$ and the result follows from Lemma 11.4.

For the upper bound, we have

$$\begin{aligned}\left|\left\langle g^{\varepsilon,\overline{\Theta_1}}_{(x_1,\xi_1)} \middle| g^{\varepsilon,\Theta_2}_{(x_2,\xi_2)} \right\rangle_{L^2(\mathbb{R}^d)}\right| &\leq \frac{(\det \Re\Theta_1 \det \Re\Theta_2)^{1/4}}{(\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} e^{-\Theta_0(x-x_2)^2/2\varepsilon} e^{-\Theta_0(x-x_1)^2/2\varepsilon}\, dx \\ &= \frac{(\det \Re\Theta_1 \det \Re\Theta_2)^{1/4}}{(\det \Theta_0)^{1/2}} \left|\left\langle g^{\varepsilon,\overline{\Theta_0}}_{(x_1,0)} \middle| g^{\varepsilon,\Theta_0}_{(x_2,0)} \right\rangle_{L^2(\mathbb{R}^d)}\right| \\ &= \frac{(\det \Re\Theta_1 \det \Re\Theta_2)^{1/4}}{(\det \Theta_0)^{1/2}} e^{-\Theta_0(x_1-x_2)^2/4\varepsilon}\end{aligned}$$

and by Parseval's Theorem

$$\begin{aligned}\left|\left\langle g^{\varepsilon,\overline{\Theta_1}}_{(x_1,\xi_1)}\middle| g^{\varepsilon,\Theta_2}_{(x_2,\xi_2)}\right\rangle_{L^2(\mathbb{R}^d)}\right| &= \left|\left\langle \mathcal{F}^\varepsilon g^{\varepsilon,\overline{\Theta_1}}_{(x_1,\xi_1)}\middle| \mathcal{F}^\varepsilon g^{\varepsilon,\Theta_2}_{(x_2,\xi_2)}\right\rangle_{L^2(\mathbb{R}^d)}\right| \\ &\leq \frac{\left(\det \Re\left(\Theta_1\right)^{-1} \det \Re\left(\Theta_2\right)^{-1}\right)^{\frac{1}{4}}}{(\pi\varepsilon)^{d/2}} \int_{\mathbb{R}^d} e^{-\Theta_0'(k-\xi_1)^2/2\varepsilon} e^{-\Theta_0'(k-\xi_2)^2/2\varepsilon}\, dk \\ &= \frac{\left(\det \Re\left(\Theta_1\right)^{-1} \det \Re\left(\Theta_2\right)^{-1}\right)^{\frac{1}{4}}}{\left(\det \Theta_0'\right)^{1/2}} \left|\left\langle g^{\varepsilon,\overline{\Theta_0'}}_{(\xi_1,0)}\middle| g^{\varepsilon,\Theta_0'}_{(\xi_2,0)}\right\rangle_{L^2(\mathbb{R}^d)}\right| \\ &= \frac{\left(\det \Re\left(\Theta_1\right)^{-1} \det \Re\left(\Theta_2\right)^{-1}\right)^{\frac{1}{4}}}{\left(\det \Theta_0'\right)^{1/2}} e^{-\Theta_0'(\xi_1-\xi_2)^2/4\varepsilon}.\end{aligned}$$

□

12 Parameters of the reference solution

We collect the parameters used for the reference solutions of Section 8.3 in Table 12.1. We recall that the potentials considered in that section are the harmonic oscillator $V(x) = x^2/2$, the Morse potential $V(x) = (1 - e^{-x})^2$ and the quartic oscillator $V(x) = x^4/4$ and that the initial datum chosen as the coherent state $g^{\varepsilon}_{(1,0)}$.

Harmonic and quartic oscillator

Parameter/ε	1e-0	1e-1	1e-2	1e-3	1e-4
Domain	[-6,6]	[-3,3]	[-2,2]	[-1.5,1.5]	[-1.25,1.25]
Time intervall	[0 25]	[0 25]	[0 25]	[0 25]	[0 25]
Gridpoints	8192	8192	8192	16384	32768
Timesteps	200000	200000	200000	400000	800000

Morse potential

Parameter/ε	1e-1	1e-2	1e-3	1e-4
Domain	[-2,5]	[-1,2]	[-1,1.5]	[-0.75,1.25]
Time intervall	[0 25]	[0 25]	[0 25]	[0 25]
Gridpoints	4096	4096	8192	16384
Timesteps	200000	200000	400000	800000

Table 12.1: Parameters of the reference solution. For $\varepsilon = 1$, the solution of the Morse potential escapes to infinity.

Table 12.2 collects the maximal error in L^2-norm over the whole time-intervall.

Potential/ε	1e-0	1e-1	1e-2	1e-3	1e-4
Harmonic oscillator	8.50e-8	2.86e-7	2.45e-6	6.02e-6	1.50e-5
Quartic oscillator	5.12e-6	4.26e-7	1.59e-6	3.30e-6	8.31e-6
Morse oscillator		1.71e-5	2.93e-6	7.25e-6	1.82e-5

Table 12.2: Maximal error of the reference solution in L^2-norm. Note that the reference is compared to a solution with half the gridpoints and half the step-size such that the actual error is lower

13 Deutsche Zusammenfassung

Die zeitabhängige Schrödingergleichung

$$i\varepsilon \frac{d}{dt}\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V(x)\psi \qquad \psi(0) = \psi_0 \in L^2(\mathbb{R}^d) \tag{13.1}$$

ist allgemein als die fundamentale Gleichung der nichtrelativistischen Quantendynamik anerkannt. Ihre Lösung, die Wellenfunktion ψ, ist eine komplexwertige, quadratintegrable Funktion auf dem Konfigurationsraum $\mathbb{R}^d$ des Systems, dessen Dimension d durch die Anzahl der Freiheitsgrade gegeben ist. Da d bereits für einfache Systeme wie etwa kleine Moleküle sehr gross werden kann, ist eine exakte Lösung der Gleichung (13.1) in der Regel weder analytisch noch numerisch erreichbar.

Unter den zahlreichen approximativen Verfahren haben sich die semiklassischen Methoden als besonders erfolgreich herausgestellt. Ihnen liegt die Beobachtung zugrunde, daß sich die Quantendynamik in makroskopischen Systemen zur klassischen Mechanik vereinfacht. Mathematisch lässt sich dieser Übergang durch den Limes $\varepsilon \to 0$ beschreiben. Zwischen den Extremen rein quantenmechanischen Verhaltens und klassischer Dynamik existiert ein Regime, in dem klassische Grössen wie Orte und Impulse zur Beschreibung der Wellenfunktion verwendet werden können.

Die vorliegende Arbeit liefert eine mathematisch rigorose Rechtfertigung für die sogenannten "Initial Value Representations" der theoretischen Chemie, eine spezielle Klasse semiklassischer Approximationen an den unitären Propagator der Gleichung (13.1). Aus mathematischer Sicht stellen diese Methoden Fourier-Integraloperatoren mit komplexwertiger Phasenfunktion dar.

Im Hauptresultat Satz 8.1 wird gezeigt, daß eine Klasse dieser Operatoren, die insbesondere die weitverbreitete Methode von Herman und Kluk sowie den sogenannten Thawed-Gaussian Propagator umfaßt, eine semiklassische Approximation an den unitären Propagator darstellen. Diese Approximationseigenschaft gilt in der Norm-Topologie der beschränkten Operatoren auf den quadratintegrablen Funktionen und kann bis zu beliebigen Ordnungen im semiklassischen Parameter ε verbessert werden. Darüber hinaus wird ein Resultat für die Ehrenfest-Zeitskala, die als die längste für semiklassische Methoden zugängliche Zeitskala gilt, gegeben.

Als wesentliche Teilresultate wird die Beschränktheit der Operatoren auf dem Raum der quadratintegrablen Funktionen im Satz 4.11 gezeigt, sowie eine asymptotische Entwicklung der Komposition Weyl-quantisierter Pseudodifferentialoperatoren und der betrachteten Klasse von Fourier-Integraloperatoren in Proposition 7.5 bewiesen.

Die Arbeit schließt mit einigen einfachen numerischen Experimenten, die die prinzipiellen Schwierigkeiten bei der Implementierung der "Initial Value Representations" aufzeigen.

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