Geometric approach to the Hamilton-Jacobi equation and global parametrices for the Schrödinger propagator

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Abstract

We construct a family of Fourier Integral Operators, defined for arbitrary large times, representing a global parametrix for the Schrödinger propagator when the potential is quadratic at infinity. This construction is based on the geometric approach to the corresponding Hamilton-Jacobi equation and thus sidesteps the problem of the caustics generated by the classical flow. Moreover, a detailed study of the real phase function allows us to recover a WKB semiclassical approximation which necessarily involves the multivaluedness of the graph of the Hamiltonian flow past the caustics.

KEYWORDS: Schrödinger equation, global Fourier Integral Operators, multivalued WKB semiclassical method, symplectic geometry.

Contents

1 Introduction and statement of the results

Let us consider the initial value problem for the Schrödinger equation:

$$\begin{cases} i\hbar\partial_t\psi(t,x) = -\dfrac{\hbar^2}{2m}\Delta\psi(t,x) + V(x)\psi(t,x), \\ \\ \psi(0,x) = \varphi(x). \end{cases} \tag{1.1}$$

where the potential $V \in C^\infty(\mathbb{R}^n;\mathbb{R})$ is assumed quadratic at infinity. In this case it is well known that the operator H in $L^2(\mathbb{R}^n)$ defined by the maximal action of $-\frac{\hbar^2}{2m}\Delta + V(x)$ is self-adjoint. Hence the Cauchy problem (1.1) considered in $L^2(\mathbb{R}^n)$ admits the unique global solution $\psi(t,x) = e^{-iHt/\hbar}\varphi(x)$, $\forall\, t \in \mathbb{R}$, $\forall\, \varphi \in L^2(\mathbb{R}^n)$.

Under the present conditions a parametrix of the propagator under the form of a semiclassical Fourier integral operator (WKB representation) has been constructed long ago by Chazarain [Ch] (for related results by the same technique see also [Fu], [Ki]; for recent related work see [MY], [Ya1], [Ya2]). The occurrence of caustics of the Hamilton-Jacobi equation makes this construction local in time; the solution at an arbitrary time $T > 0$ requires multiple compositions of the local representations. A global parametrix for the propagator has been constructed through the method of complex valued phase functions (as in [KS], [LS]), with related complex transport coefficients. A particularly convenient choice of the complex phase function (the Herman-Kluk representation) has been isolated in the chemical physics literature long ago ([H-K]). Its validity has been recently proved in [SwR] and [Ro2]). The relation between the above approaches and the underlying classical flow is however less direct than the standard WKB approximation in which the phase function solves the Hamilton-Jacobi equation.

In this paper we study the problem through the geometric approach to the Hamilton-Jacobi equation (see e.g.[CZ], [Sik86]). In Theorem 1.1 a parametrix is obtained for the propagator $U(t) := e^{iHt/\hbar}$ valid for $t \in [0,T]$, $0 < T < \infty$, under the form of a family of semiclassical *global* Fourier Integral Operators (FIO), which extend to continuous operators in $L^2(\mathbb{R}^n)$. The corresponding phase function is *real* and generates the graph of the flow of the Hamiltonian $\mathcal{H} = \frac{p^2}{2m} + V(x)$. This technique not only yields globality in time, but also helps to obtain a unified view of Fujiwara's as well as Chazarain's approaches on one side, and of the Laptev-Sigal one on the other. In Theorem 1.2 we prove that a WKB construction is still valid, necessarily multivalued because of the caustics.

We assume:

$$V(x) = \langle Lx, x\rangle + V_0(x), \quad L \in GL(n), \quad det\ L \neq 0; \tag{1.2}$$

$$V_0 \in C^\infty(\mathbb{R}^n), \quad |\partial_x^\alpha V_0(x)| \leq C_0. \tag{1.3}$$

Then the main result of the paper is:

Theorem 1.1. *Let (1.2) and (1.3) be fulfilled. Let $0 < T < \infty$ and $\varphi \in \mathcal{S}(\mathbb{R}^n)$. Then:*

$$\psi(t,x) = (2\pi\hbar)^{-n} \sum_{j=0}^{\infty} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}\hbar^j b_j(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy + O(\hbar^\infty) \tag{1.4}$$

Here:

$$k > C\ T^4 \sup_{|\alpha|+|\beta|\geq 2}\ \sup_{(x,p)\in\mathbb{R}^{2n}} |\partial_x^\alpha \partial_p^\beta \mathcal{H}(x,p)|^2 \tag{1.5}$$

for some $C > 0$. Moreover the following assertions hold:
(1) S generates the graph Λ_t of the Hamiltonian flow $\phi^t_{\mathcal{H}} : T^\star\mathbb{R}^n \to T^\star\mathbb{R}^n\ \forall t \in [0,T]$:

$$\begin{aligned}\Lambda_t &:= \{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid (x,p) = \phi^t_{\mathcal{H}}(y,\eta)\} \\ &= \{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x S,\ y = \nabla_\eta S,\ 0 = \nabla_\theta S\}\end{aligned} \tag{1.6}$$

(2) $S \in C^\infty([0,T]\times\mathbb{R}^{2n}\times\mathbb{R}^k;\mathbb{R})$ and has the expression:

$$\begin{aligned} S &= \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle Q(t)\theta,\theta\rangle + \langle v(t,x,\eta), \theta + f(t,x,\theta)\rangle + \langle \nu(t,x,\eta,\theta),\theta\rangle \\ &+ g(t,x,\eta,\theta). \end{aligned} \tag{1.7}$$

Here $f(t,x,\theta) : [0,T]\times\mathbb{R}^n\times\mathbb{R}^k \to \mathbb{R}^k$, $\nu(t,x,\eta,\theta) : [0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k \to \mathbb{R}^k$, $g(t,x,\eta,\theta)$: $[0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k \to \mathbb{R}$ and $C_{\alpha\beta\sigma}(T) > 0$ are such that

$$\sup_{[0,T]\times\mathbb{R}^{2n+k}} [|\partial_x^\alpha\partial_\theta^\sigma f(t,x,\eta,\theta)| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma g(t,x,\eta,\theta)| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma \nu(t,x,\eta,\theta)|] \leq C_{\alpha\beta\sigma}(T).$$

The function $(x,\eta) \mapsto v(t,x,\eta) : \mathbb{R}^n\times\mathbb{R}^n \to \mathbb{R}$ is linear $\forall t \in \mathbb{R}$, and $t \mapsto Q(t) : [0,T] \to GL(k)$ with $Q(0) = 0$.

(2) The transport coefficients $b_j : j = 0, \ldots$ are determined by the first order PDE:

$$\begin{cases} \partial_t b_0 + \frac{1}{m}\nabla_x S\ \nabla_x b_0 + \frac{1}{2m}\Delta_x S\ b_0(t,x,\eta,\theta) = \Theta_N, \\ b_0(0,x,\eta,\theta) = \rho(\theta). \end{cases} \quad j = 0 \tag{1.8}$$

$$\begin{cases} \partial_t b_j + \dfrac{1}{m}\nabla_x S\ \nabla_x b_j + \dfrac{1}{2m}\Delta_x S\ b_j - \dfrac{i}{2m}\Delta_x b_{j-1} = 0, \\ b_j(0,x,\eta,\theta) = 0, \quad \rho(\theta) \in \mathcal{S}(\mathbb{R}^k;\mathbb{R}^+),\ \|\rho\|_{L^1} = 1. \end{cases} \quad j \geq 1 \tag{1.9}$$

Here $\Theta_N \in C_b^\infty(\mathbb{R}^{2n+k};\mathbb{R})$ *is arbitrary within the requirement:*

$$\begin{aligned}&\Pi^\alpha \Theta_N \in C_b^\infty(\mathbb{R}^{2n+k};\mathbb{R}),\ 0\le \alpha \le N;\\ &\Pi\Theta_N := \mathrm{div}\left(\Theta_N \frac{\nabla_\theta S}{|\nabla_\theta S|^2}\right).\end{aligned}$$

(3) $\forall\, 0 \le t \le T$, $0 \le T < +\infty$, *the expansion (1.4) generates an* L^2 *parametrix of the propagator* $U(t) = e^{iHt/\hbar}$*: each term is a continuos FIO on* $\mathcal{S}(\mathbb{R}^n)$ *denoted* $B_j(t)$, $j = 0, 1, \ldots,$ *which admits a continuous extension to* $L^2(\mathbb{R}^n)$, *and:*

$$e^{iHt/\hbar} = \sum_{j=0}^{\infty} B_j(t) + O(\hbar^\infty). \tag{1.10}$$

The notation $O(\hbar^\infty)$ *means:*

$$\|R_N(t)\|_{L^2\to L^2} \le C_N(T)\hbar^{N+1}, \forall\, N \ge 0,\ \forall\, t \in [0,T], \quad R_N(t) := U(t) - \sum_{j=0}^{N} B_j(t).$$

Moreover, the expansion (1.10) does not depend on ρ *provided* $\|\rho\|_{L^1} = 1$*. Namely, if* $\rho_1 \neq \rho_2$*:*

$$\sum_{j=0}^{N} B_j[\rho_1](t) - \sum_{j=0}^{N} B_j[\rho_2](t) = O(\hbar^{N+1}).$$

By applying the stationary phase theorem to the oscillatory integral (1.4), the integration over the auxiliary parameters θ can be eliminated and the WKB approximation to the evolution operator is recovered, necessarily multivalued on account of the caustics.

Theorem 1.2. *Let* $V(x) = \frac{1}{2}|x|^2 + V_0(x)$ *with* $\sup_{x\in\mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1$*; let* $\widehat{\varphi}_\hbar(\eta)$ *be the* $\hbar$*-Fourier transform of the initial datum* φ*. Then* $\forall\, t \in [0,T]$, $t \neq (2\tau+1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$, *there exists a finite open partition* $\mathbb{R}^n \times \mathbb{R}^n = \bigcup_{\ell=1}^{\mathcal{N}} D_\ell$ *such that the solution of (1.1) can be represented as:*

$$\psi(t,x) = \int_{\mathbb{R}^n} \widehat{U}_\hbar(t,x,\eta)\ \widehat{\varphi}_\hbar(\eta)\ d\eta, \quad 0 \le t \le T, \quad t \neq (2\tau+1)\frac{\pi}{2}$$

$$\widehat{U}_\hbar(t,x,\eta)\Big|_{D_\ell} = \sum_{\alpha=1}^{\ell} e^{\frac{i}{\hbar}S_\alpha(t,x,\eta)}\ |\mathrm{det}\nabla^2_\theta S(t,x,\eta,\theta^\star_\alpha(t,x,\eta))|^{-\frac{1}{2}} e^{\frac{i\pi}{4}\sigma_\alpha} b_{\alpha,0}(t,x,\eta) + O(\hbar) \tag{1.11}$$

$$S_\alpha := S(t,x,\eta,\theta^\star_\alpha(t,x,\eta)),\ b_{\alpha,0} := b_0(t,x,\eta,\theta^\star_\alpha(t,x,\eta)),\ \sigma_\alpha := sgn\nabla^2_\theta S(t,x,\eta,\theta^\star_\alpha(t,x,\eta))$$

where $\mathcal{N}$ *is a* $t-$*dependent natural and:*

(i) On each D_ℓ *the equation* $0 = \nabla_\theta S(t,x,\eta,\theta)$ *has* ℓ *smooth solutions* $\theta^\star_\alpha(t,x,\eta)$, $1 \le \alpha \le \ell$.

(ii) Any function $S_\alpha(t,x,\eta)$ solves locally the Hamilton-Jacobi equation:

$$\frac{|\nabla_x S_\alpha|^2}{2m}(t,x,\eta) + V(x) + \partial_t S_\alpha(t,x,\eta) = 0$$

(iii) An explicit upper bound on the t-dependent natural $\mathcal{N}$ is computed in (2.68).

Example In the harmonic oscillator case $V(x) = \frac{1}{2}x^2$ and the phase function is exactly quadratic $S(t,x,\eta,\theta) = \langle x,\eta\rangle - \frac{t}{2}(\eta^2 + x^2) + \langle v(t,x,\eta),\theta\rangle + \langle Q(t)\theta,\theta\rangle$ It admits a unique smooth global critical point $\theta^\star(t,x,\eta)$ on $(x,\eta) \in \mathbb{R}^{2n}$ for $t \in [0,T]$, $t \neq (2\tau+1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$. Hence the series (1.11) reduces to just one term conciding with the well known Mehler formula:

$$\psi(t,x) = \int_{\mathbb{R}^n} e^{\frac{i}{\hbar\cos(t)}\left(\langle x,\eta\rangle - \frac{\sin(t)}{2}(\eta^2+x^2)\right)} \frac{1}{\cos(t)}\hat{\varphi}_\hbar(\eta)d\eta$$

Remarks

1. The phase function is constructed (Section 2) through the Amann-Conley-Zehnder reduction technique of the action functional ([AZ], [CZ],[Car]). Namely:

$$S(t,x,\eta,\theta) = \langle x,\eta\rangle + \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - H(\gamma^x(s),\eta+\gamma^p(s))]\; ds\Big|_{\gamma(t,x,\theta)(\cdot)} \tag{1.12}$$

where the curves $\Gamma(t,x,\theta) = (\gamma^x(t,x,\theta)(s), \gamma^p(t,x,\theta)(s))$ are parametrized as follows:

$$\Gamma(t,x,\theta) := \begin{cases} \gamma^x(t,x,\theta)(s) = x - \int_s^t \phi^x(t,x,\theta)(\tau)\; d\tau, \quad \phi^x = \theta^x(\cdot) + f^x(t,x,\theta)(\cdot), \\ \gamma^p(t,x,\theta)(s) = \int_0^s \phi^p(t,x,\theta)(\tau)\; d\tau, \quad \phi^p = \theta^p(\cdot) + f^p(t,x,\theta)(\cdot) \end{cases} \tag{1.13}$$

Here $\theta \in \mathbb{P}_M L^2([0,T];\mathbb{R}^{2n}) \simeq \mathbb{R}^k$ ($\mathbb{P}_M$ is the finite dimensional Fourier orthogonal projector, $k = 2n(2M+1)$) so that the parameters θ can be identified with the finite Fourier components of the derivatives of the curves γ. (1.12) represents a global generating function if k fulfills the lower bound (1.5). In turn, the functions $(f^x,f^p) : [0,T]\times\mathbb{R}^n\times\mathbb{P}_M L^2 \to \mathbb{Q}_M L^2 \times \mathbb{Q}_M L^2$ are determined by a fixed point functional equation, essentially the $\mathbb{Q}_M$ projection of the Hamilton equations (Section 2.3). The parametrization (1.6) entails that S is a smooth solution of the problem:

$$\begin{cases} \frac{|\nabla_x S|^2}{2m}(t,x,\eta,\theta) + V(x) + \partial_t S(t,x,\eta,\theta) = 0, \\ S(0,x,\eta,\theta) = \langle x,\eta\rangle; \quad \nabla_\theta S(t,x,\eta,\theta) = 0. \end{cases} \tag{1.14}$$

2. Any function $S(t,x,\eta,\theta)$ solving (1.14), i.e. the Hamilton-Jacobi equation under the stationarity constraint $\nabla_\theta S = 0$, is the central object to determine the so called *geometrical solutions of the Hamilton-Jacobi equation* (see for example the recent works [Car], [B-C]). Global generating functions are clearly not unique and this is due to the presence of the θ-auxiliary parameters. Uniqueness holds instead for the geometry of set of critical points:

$$\Sigma_S := \{(x,\eta,\theta) \in \mathbb{R}^{2n+k} \mid \nabla_\theta S(t,x,\eta,\theta) = 0\}$$

which does not depend on S because it is globally diffeomorphic to Λ_t; a detailed study of Σ_S is done in Section 2. We prove (Section 3) that symbols coinciding on Σ_S generate semiclassical Fourier Integral Operators differing only by terms $O(\hbar^\infty)$. This will allow us to select symbols in such a way to make essentially trivial the proof of the L^2 continuity of the associated operator.

3. The symbol b_0 solving the geometrical version (1.8) of the transport equation is

$$b_0(t,x,\eta,\theta) = \exp\left\{-\frac{1}{2m}\int_0^t \Delta_x S(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)d\tau\right\}\rho(\theta) \tag{1.15}$$

If $T_2 > T_1$, then $k(T_2) > k(T_1)$ so that $\Gamma(T_1,x,\theta) \subset \Gamma(T_2,x,\theta)$. In the limit $T \to \infty$, $\theta \to \phi \in L^2(\mathbb{R}^+;\mathbb{R}^{2n})$ and we get the simplified functional (still well defined):

$$b_0(t,x,\phi) = \exp\left\{\frac{1}{2m}\int_0^t \Delta_x V(x - \int_\tau^t \phi^x(\lambda)\ d\lambda)d\tau\right\}\rho(\phi) \tag{1.16}$$

This corresponds to the zero-th order symbol of the Laptev-Sigal construction [LS]:

$$v_0(t,y,\eta) = \exp\left\{\frac{1}{2m}\int_0^t \Delta_x V(x^\tau(y,\eta))d\tau\right\}.$$

Namely, the functional is the same, but is evaluated on the classical curves (with initial conditions $x^0(y,\eta) = y$, $p^0(y,\eta) = \eta$) instead of all the free curves used in (1.16), with regularity H^1 and boundary condition $\gamma^x(t,x,\phi)(t) = x$.

4. For potentials in the class (1.2) and $0 \le t \le T$ small enough no caustics develop, and there is a unique smooth solution $\theta^\star(t,x,\eta)$ for $(x,\eta) \in \mathbb{R}^{2n}$. The stationary phase theorem yields the 0-th order approximation to the integral (1.4):

$$\widehat{U}_\hbar^{(0)}(t,x,\eta) = e^{\frac{i}{\hbar}S(t,x,\eta,\theta^\star)}|\det\nabla_\theta^2 S(t,x,\eta,\theta^\star)|^{-\frac{1}{2}}e^{\frac{i\pi}{4}\sigma}b_0(t,x,\eta,\theta^\star) + O(\hbar) \tag{1.17}$$

which coincide with the WKB semiclassical approximation. This fact suggests a relationship, at any order in $\hbar$, between the present construction and those of Chazarain [Ch] and Fujiwara [Fu]. This is the contents of Theorem 4.2.

5. The first three assertions of Theorem 1.2 represent the counterpart (in the η variables) of a result of Fujiwara [Fu], valid under the additional assumption that the number of classical curves connecting boundary data is finite.

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2 Generating functions for the graph of the Hamiltonian flow

2.1 Lagrangian submanifolds and global generating functions

Adopting standard notations and terminology (see e.g.[We]), we denote by $\omega = dp \wedge dx = \sum_{i=1}^{n} dp_i \wedge dx^i$ the 2–form on $T^\star\mathbb{R}^n$ that defines its natural symplectic structure. As usual, a diffeomorphism $\mathcal{C} : T^\star\mathbb{R}^n \to T^\star\mathbb{R}^n$ is a *canonical transformation* if the pull back of the symplectic form is preserved, $\mathcal{C}^\star\omega = \omega$.
We say that $L \subset T^\star\mathbb{R}^n$ is a *Lagrangian submanifold* if $\omega|_L = 0$ and $\dim L = n = \frac{1}{2}\dim T^\star\mathbb{R}^n$. In a natural way, a symplectic structure $\bar{\omega}$ on $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \cong T^\star(\mathbb{R}^n \times \mathbb{R}^n)$ is the twofold pull–back of the standard symplectic 2–form on $T^\star\mathbb{R}^n$ defined as $\bar{\omega} := pr_2^\star\omega - pr_1^\star\omega = dp_2 \wedge dx_2 - dp_1 \wedge dx_1$. Similarly, $\Lambda \subset T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$ is called a Lagrangian submanifold of $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$ if $\bar{\omega}|_\Lambda = 0$ and $\dim(\Lambda) = 2$n.
A Hamiltonian is a C^2-function $\mathcal{H} : T^\star\mathbb{R}^n \to \mathbb{R}$ and its flow is the one-parameter group of canonical transformations $\phi^t_{\mathcal{H}} : U \subseteq T^\star\mathbb{R}^n \to T^\star\mathbb{R}^n$ solving Hamilton's equations $\dot{\gamma} = J\nabla\mathcal{H}(\gamma)$ (J the unit symplectic matrix) with initial conditions $\gamma(0) = (x_0, p_0) \in U$.
The Hamilton-Helmholtz functional:

$$A[(\gamma^x, \gamma^p)] := \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - \mathcal{H}(\gamma^x(s), \gamma^p(s))]\, ds \tag{2.1}$$

is well defined and continuous on the path space $H^1([0,t]; T^\star\mathbb{R}^n)$. The action functional:

$$\mathcal{A}[\gamma^x] := \int_0^t \mathcal{L}(\gamma^x(s), \dot{\gamma}^x(s))\, ds \tag{2.2}$$

is defined on $H^1([0,t]; \mathbb{R}^n)$. In this paper we consider $\mathcal{H} = \dfrac{p^2}{2m} + V(x)$, so that the Legendre transform guarantees the corrispondence of the stationary curves of these two functionals.

Definition 2.1. *A global generating function for a Lagrangian submanifold $L \subset T^\star\mathbb{R}^n$ is a C^2 function $S : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ such that*

◇ $L = \{(x,p) \in T^\star\mathbb{R}^n |\ p = \nabla_x S(x,\theta),\ \ 0 = \nabla_\theta S(x,\theta)\ \}$,

◇ *rank* $\left(\nabla^2_{x\theta} S\ \nabla^2_{\theta\theta} S\right)\Big|_L = \max.$

Similarly, a global generating function for a Lagrangian submanifold $\Lambda \subset T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$ *is a* C^2 *map* $S : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ *such that*

◇ $\Lambda = \{(x,p;y,\eta) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n |\ p = \nabla_x S(x,\eta,\theta),\ \ y = \nabla_\eta S(x,\eta,\theta),\ \ 0 = \nabla_\theta S\ \}$,

◇ *rank* $\left(\nabla^2_{x\theta} S\ \nabla^2_{\eta\theta} S\ \nabla^2_{\theta\theta} S\right)\Big|_\Lambda = \max.$

It is important to remark that the following set:

$$\Sigma_S := \{(x,\eta,\theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \mid 0 = \nabla_\theta S(x,\eta,\theta)\} \tag{2.3}$$

is a submanifold of $\mathbb{R}^{2n+k}$ and it is diffeomorphic to Λ.

We focus our attention on the graphs of a Hamiltonian flow $\phi^t_{\mathcal{H}} : T^\star\mathbb{R}^n \to T^\star\mathbb{R}^n$, which correspond to a family of Lagrangian submanifolds in $T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n$:

$$\Lambda_t := \left\{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid (x,p) = \phi^t_{\mathcal{H}}(y,\eta)\right\}$$

An important object in what follows is the family of global generating functions:

$$\Lambda_t = \{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x S, \quad y = \nabla_\eta S, \quad 0 = \nabla_\theta S(t,x,\eta,\theta)\}$$

to be explicitly constructed for arbitrarily large times in the next Section. As is known, this technical tool has been developed in the framework of symplectic geometry and variational analysis (see [AZ], [CZ], [Cha], [LSik], [Vit], [Sik86], [Sik]) to sidestep the locality in time generated by the occurrence of caustics.

2.2 Generating function with infinitely many parameters

In the following we mainly review the construction of a generating function with infinitely many parameters described in [Car]. We begin by the following simple result (see [We]):

Lemma 2.2. *Let us consider the Hamilton-Helmholtz functional* $A[\cdot]$ *as in (2.1). A curve* $\gamma \in \Gamma^{(0)} := \{\gamma \in H^1([0,t]; T^\star\mathbb{R}^n) \mid \gamma^p(0) = 0,\ \gamma^x(t) = x\}$ *satisfies Hamilton's equations with boundary conditions:*

$$\dot\gamma = J\nabla\mathcal{H}(\gamma), \quad \gamma^p(0) = 0, \quad \gamma^x(t) = x$$

if and only if the following stationarity condition of variational type holds:

$$\frac{DA}{D\gamma}(\gamma)[v] = 0 \quad \forall v \in T\Gamma^{(0)}$$

Proof. By computing the Gâteaux derivative of the functional, we get:

$$\frac{DA}{D\gamma}(\gamma)[v] = \int_0^t [\dot{\gamma} - J\nabla\mathcal{H}(\gamma)](s)v(s)\ ds + \gamma^p(s)v^x(s)|_0^t \quad \forall v \in T\Gamma^{(0)}.$$

Now use the boundary condition $\gamma^p(0) = 0$ and recall that for $T\Gamma^{(0)}$ it must be $v^x(t) = 0$. The result is proved. □

The above Lemma has an important consequence: it allows us to introduce the notion of generating function with infinitely many parameters.
First of all, it is easy to observe that the set of curves

$$\gamma(t,x,\phi)(s) := \left(x - \int_s^t \phi^x(\tau)d\tau, \int_0^s \phi^p(\tau)d\tau\right) \qquad \phi \equiv (\phi^x, \phi^p) \tag{2.4}$$

gives a parametrization of the path space $\Gamma^{(0)}$ introduced in the previous lemma, namely:

$$\Gamma^{(0)}(t,x,\phi) := \left\{\gamma(t,x,\phi)(\cdot) \mid \phi \in L^2([0,T];\mathbb{R}^{2n})\right\}$$

Second, we define the functional with *infinitely many parameters* specified by $\phi \in L^2([0,T];\mathbb{R}^{2n})$ in the following way:

Definition 2.3.

$$\mathcal{S}(t,x,\eta,\phi) := \langle x,\eta\rangle + \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - H(\gamma^x(s),\eta+\gamma^p(s))]\ ds\Big|_{\gamma(\cdot)=\gamma(t,x,\phi)(\cdot)} \tag{2.5}$$

Remark
Introducing the traslated curves $\zeta = (\zeta^x,\zeta^p) := (\gamma^x, \eta+\gamma^p)$, it is easy to see that the functional (2.5) admits the equivalent representation

$$\mathcal{S}(t,x,\eta,\phi) = \langle\zeta^x(0),\eta\rangle + \int_0^t \zeta^p(s)\dot{\zeta}^x(s) - H(\zeta^x(s),\zeta^p(s))\ ds\Big|_{\zeta(\cdot)=\zeta(t,x,\phi)(\cdot)}$$

where now $\zeta^x(t) = x$ and $\zeta^p(0) = \eta$.

Let us now make our assumptions on the Hamiltonian $\mathcal{H}$ more precise:

Definition 2.4.

$$\mathcal{H}(x,p) = \frac{p^2}{2m} + V(x) = \frac{p^2}{2m} + \langle Lx,x\rangle + V_0(x) \tag{2.6}$$

where $V_0 \in C^\infty(\mathbb{R}^n)$, $L \in GL(n)$, *and*

$$|\partial_x^\alpha V_0(x)| \le C_0,$$

This allows us to look more closely at the structure of the generating function:

Lemma 2.5. *The functional $\mathcal{S}$ admits the representation:*

$$\mathcal{S}(t,x,\eta,\phi) \;=\; \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle R(t)\phi,\phi\rangle + \langle v(t,x,\eta),\phi\rangle + \sigma(t,x,\phi). \tag{2.7}$$

Here $v(t,x,\eta)$ has a linear dependence with respect to (x,η) variables, and $\sigma(t,x,\phi)$ is bounded with respect to (x,ϕ).

Proof. It is easy to see that:

$$\begin{aligned}
\mathcal{S} &= \langle x,\eta\rangle + \int_0^t \left(\int_0^s \phi^p(\tau)d\tau\right)\phi^x(s)ds \\
&- \int_0^t \frac{1}{2m}\left(\eta + \int_0^s \phi^p(\tau)d\tau\right)^2 + L\left(x - \int_s^t \phi^x(\tau)d\tau\right), \left(x - \int_s^t \phi^x(\tau)d\tau\right) ds \\
&- \int_0^t V_0\left(x - \int_s^t \phi^x(\tau)d\tau\right) ds \\
&= \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle R(t)\phi,\phi\rangle + \langle v(t,x,\eta),\phi\rangle + \sigma(t,x,\phi)
\end{aligned} \tag{2.8}$$

where

$$\begin{aligned}
\langle R(t)\phi,\phi\rangle &:= \int_0^t \left(\int_0^s \phi^p(\tau)d\tau\phi^x(s) - \frac{1}{2m}\left(\int_0^s \phi^p(\tau)d\tau\right)^2 - L\int_s^t \phi^x(\tau)d\tau\int_s^t \phi^x(\tau)d\tau\right) ds \\
\langle v(t,x,\eta),\phi\rangle &:= \int_0^t \left(-\frac{\eta}{m}\int_0^s \phi^p(\tau)d\tau + 2Lx\int_s^t \phi^x(\tau)d\tau\right) ds \\
\sigma(t,x,\phi) &:= -\int_0^t V_0\left(x - \int_s^t \phi^x(\tau)d\tau\right)\, ds
\end{aligned} \tag{2.9}$$

The boundedness of σ is immediate:

$$\sup_{(x,\phi)\in\mathbb{R}^n\times L^2} |\sigma(t,x,\phi)| \le t \sup_{z\in\mathbb{R}^n} |V_0(z)|$$

Finally, we consider the orthonormal basis of L^2, $e_\alpha(s) = \frac{1}{\sqrt{T}}e^{\frac{2\pi}{T}i\alpha s}$, $\alpha\in\mathbb{Z}$ and the corresponding Fourier expansion $\phi(s) = \sum_{\alpha\in\mathbb{Z}}\phi^{(\alpha)}e_\alpha(s)$. This entails the identification $\phi(s) \equiv \{\phi^{(\alpha)}\}_{\alpha\in\mathbb{Z}} \in \ell^2$ under the usual norm $|\phi| = \sum_\alpha |\phi^{(\alpha)}|^2$ generated by the scalar product $\langle\psi,\phi\rangle = \sum_\alpha \psi^{(\alpha)}\phi^{(\alpha)}$.

□

Proposition 2.6. *The graph of the Hamiltonian flow*

$$\Lambda_t := \left\{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid (x,p) = \phi^t_{\mathcal{H}}(y,\eta)\right\}$$

is generated by $\mathcal{S}$*:*

$$\Lambda_t = \left\{ (y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x \mathcal{S}, \quad y = \nabla_\eta \mathcal{S}, \quad 0 = \frac{D\mathcal{S}}{D\phi} \right\}$$

Proof. The first component of the stationarity equation $0 = \dfrac{D\mathcal{S}}{D\phi}$ reads:

$$0 = \frac{D\mathcal{S}}{D\phi^p}(\phi)[v^p] = \int_0^t \left(\int_0^s v^p(\tau)d\tau \right) \phi^x(s) - \frac{1}{m} \left(\eta + \int_0^s \phi^p(\tau)d\tau \right) \left(\int_0^s v^p(\tau)d\tau \right) ds$$

for all $v^p \in L^2$. This is satisfied if and only if

$$\phi^x(s) = \frac{1}{m} \left(\eta + \int_0^s \phi^p(\tau)\ d\tau \right) \tag{2.10}$$

that is

$$\dot\gamma^x(t,x,\phi)(s) = \frac{1}{m} \left(\eta + \gamma^p(t,x,\phi)(s) \right) \tag{2.11}$$

On the other hand, the second equation reads:

$$0 = \frac{D\mathcal{S}}{D\phi^x}(\phi)[v^x] = \int_0^t \left(\int_0^s \phi^p(\tau)d\tau \right) v^x(s) + \nabla V \left(x - \int_s^t \phi^x(\tau)d\tau \right) \int_s^t v^x(\tau)d\tau\ ds$$

for all $v^x \in L^2$. Integrating by parts, we get

$$\begin{aligned} 0 &= \int_0^t \phi^p(s)ds \int_0^t v^x(\tau)d\tau - \int_0^t \phi^p(s) \int_0^s v^x(\tau)d\tau + \nabla V \left(x - \int_s^t \phi^x(\tau)d\tau \right) \int_s^t v^x(\tau)d\tau\ ds \\ &= \int_0^t \phi^p(s) \int_s^t v^x(\tau)d\tau + \nabla V \left(x - \int_s^t \phi^x(\tau)d\tau \right) \int_s^t v^x(\tau)d\tau\ ds. \end{aligned}$$

This entails:

$$\phi^p(s) = -\nabla V \left(x - \int_s^t \phi^x(\tau)d\tau \right) \tag{2.12}$$

that is equivalent to

$$\dot\gamma^p(t,x,\phi)(s) = -\nabla_x V(\gamma^x(t,x,\phi)(s)). \tag{2.13}$$

By a simple computation and (2.10) we get:

$$\begin{aligned} \nabla_\eta \mathcal{S} &= x - t\frac{\eta}{m} - \frac{1}{m} \int_0^t \int_0^s \phi^p(\tau)d\tau ds = x - t\frac{\eta}{m} - \int_0^t \left(\phi^x(s) - \frac{1}{m}\eta \right) ds \\ &= x - t\frac{\eta}{m} - \int_0^t \phi^x(s)ds + t\frac{\eta}{m} = x - \int_0^t \phi^x(s)ds = \gamma^x(t,x,\phi)(0) = y \end{aligned}$$

Finally, by (2.12), we can complete the verification:

$$\begin{aligned} \nabla_x \mathcal{S} &= \eta - \int_0^t \nabla V \left(x - \int_s^t \phi^x(\tau)d\tau \right) ds \\ &= \eta + \int_0^t \phi^p(s)ds = \eta + \gamma^p(t,x,\phi)(t) = p \end{aligned}$$

□

The following statement is a direct consequence of the above result:

Proposition 2.7. *The Hamilton-Jacobi equation is solved on the stationarity points* $0 = \dfrac{D\mathcal{S}}{D\phi}$*; more precisely* $\mathcal{S}$ *is a smooth solution of the problem:*

$$\begin{cases} \partial_t \mathcal{S}(t,x,\eta,\phi) + \dfrac{|\nabla_x \mathcal{S}|^2}{2m}(t,x,\eta,\phi) + V(x) = 0, \quad (t,x) \in \mathbb{R}^+ \times \mathbb{R}^n \\ \mathcal{S}(0,x,\eta,\phi) = \langle x, \eta \rangle, \quad \dfrac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi) = 0. \end{cases} \tag{2.14}$$

For the proof we refer to [Car] (sections 3 and 4).

Remark 2.8. *As we have seen in Proposition 2.6, fix* $t \in [0,T]$ *and define the map*

$$G_t : \mathbb{R}^{2n} \times L^2([0,T];\mathbb{R}^{2n}) \to L^2([0,T];\mathbb{R}^{2n}) \tag{2.15}$$

$$G_t(x,\eta,\phi^x,\phi^p) := \left(\frac{\eta}{m} + \frac{1}{m} \int_0^s \phi^p(\tau)\ d\tau, -\nabla V \left(x - \int_s^t \phi^x(\tau) d\tau \right) \right). \tag{2.16}$$

Then, the fixed point equation on $L^2([0,T];\mathbb{R}^{2n})$*:*

$$\phi = G_t(x,\eta,\phi) \tag{2.17}$$

is equivalent to the stationarity equation

$$0 = \frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi)$$

On the other hand, the solution of this equation determines the curves

$$\zeta(t,x,\phi)(s) := \left(x - \int_s^t \phi^x(\tau) d\tau, \eta + \int_0^s \phi^p(\tau) d\tau \right) \qquad \phi \equiv (\phi^x, \phi^p) \tag{2.18}$$

solving the Hamilton's equations $\dot{\zeta} = J\nabla H(\zeta)$ *with boundary conditions* $\zeta^x(t) = x$, $\zeta^p(0) = \eta$.

The following result deals with some topological properties for the set of the solutions. Let:

$$t_{\alpha,\beta} := \frac{\pi}{2\sqrt{\lambda_\alpha}}(2\beta+1), \ \alpha = 1,2,\dots,n; \quad \beta \in \mathbb{N} \tag{2.19}$$

$$\lambda(x,\eta) := \sqrt{1 + |x|^2 + |\eta|^2} \tag{2.20}$$

where $\lambda_\alpha : \alpha = 1,2,\dots,n$ are the eigenvalues of $L + L^\dagger$. Remark that $t_{\alpha,\beta}$ are just the resonant times of the hamiltonian flow generated by $\mathcal{H}_0 := \dfrac{p^2}{2m} + \langle Lx, x \rangle$.

Proposition 2.9. *There are* $D(T) < +\infty$, $K_2(T) < +\infty$, $K_1(t) < +\infty$ *such that the solutions of equation (2.17) fulfill the estimates:*

$$\|\phi\|_{L^2} \ > \ K_2(T)\lambda(x,\eta) \quad \forall t \in]0,T], \qquad |x|^2 + |\eta|^2 > D(T)^2; \tag{2.21}$$

$$\|\phi\|_{L^2} \ \leq \ K_1(t)\lambda(x,\eta) \quad \forall t \neq t_{\alpha,\beta}, \quad \forall (x,\eta) \in \mathbb{R}^{2n}. \tag{2.22}$$

Moreover, there is $E(t) < +\infty$ such that the difference of any two solutions ϕ, ψ of (2.17) fulfills the estimate

$$\|\phi - \psi\|_{L^2} \leq E(t) \quad \forall t \neq t_{\alpha,\beta}, \quad \forall (x,\eta) \in \mathbb{R}^{2n}. \tag{2.23}$$

Proof. We begin by remarking that the equation (2.17)

$$(\phi^x, \phi^p) = \left(\frac{\eta}{m} + \frac{1}{m}\int_0^s \phi^p(\tau)\, d\tau, -\nabla V\left(x - \int_s^t \phi^x(\tau) d\tau\right)\right),$$

can be rewritten as

$$\phi - \mathcal{L}(t,\phi) = \Psi_0(t,x,\eta) + \Psi_1(t,x,\phi) \tag{2.24}$$

where

$$\begin{aligned} \mathcal{L}(t,\phi) &:= \left(\frac{1}{m}\int_0^s \phi^p(\tau)\, d\tau, (L+L^\dagger)\int_s^t \phi^x(\tau)d\tau\right) \\ \Psi_0(t,x,\eta) &:= \left(\frac{\eta}{m}, -(L+L^\dagger)x\right) \\ \Psi_1(t,x,\phi) &:= \left(0, -\nabla V_0\left(x - \int_s^t \phi^x(\tau)d\tau\right)\right) \end{aligned} \tag{2.25}$$

To prove the inequality (2.21), remark that the non-degeneracy of $L + L^\dagger$ entails the lower and upper bounds:

$$W_0(T)\lambda(x,\eta) \leq \|\Psi_0(t,x,\eta)\|_{L^2} = T^{\frac{1}{2}}\left(\frac{|\eta|^2}{m^2} + |(L+L^\dagger)x|^2\right)^{\frac{1}{2}} \leq C_0(T)\lambda(x,\eta). \tag{2.26}$$

Here $W_0(T) := T^{\frac{1}{2}}\mu_M$, $C_0(T) := T^{\frac{1}{2}}; \mu_m$ and μ_M, μ_m are the maximum and the minimum eigenvalue of the matrix:

$$\mathbf{X} = \begin{pmatrix} \frac{1}{m^2}I & 0 \\ 0 & (L+L^\dagger)^2 \end{pmatrix}$$

respectively. Moreover,

$$\|\Psi_1(t,x,\phi)\|_{L^2} = \left(\int_0^T |\nabla V_0\left(x - \int_s^t \phi^x(\tau)d\tau\right)|^2 ds\right)^{\frac{1}{2}} \leq T^{\frac{1}{2}}\|\nabla V_0\|_{C^0} =: C_1(T) \tag{2.27}$$

Now set $\mathcal{M}(t,\phi) := \phi - \mathcal{L}(t,\phi)$. Hence the solutions of the equation (2.24) fulfill the estimate:

$$\begin{aligned} \sup_{t\in[0,T]} \|\mathcal{M}(t,\cdot)\|_{L^2 \mapsto L^2}\|\phi\|_{L^2} &\geq \|\mathcal{M}(t,\phi)\|_{L^2} = \|\Psi_0(t,x,\eta) + \Psi_1(t,x,\phi)\|_{L^2} \\ &\geq W_0(T)\lambda(x,\eta) - C_1(T) \end{aligned} \tag{2.28}$$

For $|x|^2 + |\eta|^2 > D(T)^2$ we have $W_0(T)\lambda(x,\eta) - C_1(T) > \dfrac{W_0(T)}{2}\lambda(x,\eta)$, and this implies

$$\|\phi\|_{L^2} > \left(\sup_{t\in[0,T]} \|\mathcal{M}(t,\cdot)\|_{L^2\mapsto L^2}\right)^{-1} \frac{W_0(T)}{2}\lambda(x,\eta) =: K_2(T)\lambda(x,\eta)$$

Now consider equation (2.24) in the particular case of $V_0 = 0$ (so that the Hamiltonian is $\mathcal{H}_0 := \frac{p^2}{2m} + \langle Lx, x\rangle$). It becomes:

$$\phi - \mathcal{L}(t,\phi) = \Psi_0(t,x,\eta) \qquad (x,\eta) \in \mathbb{R}^n \times \mathbb{R}^n \tag{2.29}$$

The explicit representation of the flow for the harmonic oscillator is $\phi^s_{\mathcal{H}_0}(\zeta^x_0, \zeta^p_0) = e^{sU}(\zeta^x_0, \zeta^p_0)$ where

$$\mathbf{U} = \begin{pmatrix} 0 & \frac{I}{m} \\ -(L + L^{\dagger}) & 0 \end{pmatrix}$$

It is easy to prove that outside the resonant times $t_{\alpha,\beta}$ the flow can be globally inverted with respect to the boundary conditions (x, η), namely: $\zeta^x(s) = \zeta^x(t,x,\eta)(s)$ and $\zeta^p(s) = \zeta^p(t,x,\eta)(s)$. By recalling Remark 2.8, this fact is equivalent to the existence of a unique global smooth solution $\phi^{\star}_0(t,x,\eta)$ for equation (2.29). This argument works $\forall (x,\eta) \in \mathbb{R}^n \times \mathbb{R}^n$. In the particular case $x = \eta = 0$ (2.29) reduces to:

$$\mathcal{M}(t,\phi) := \phi - \mathcal{L}(t,\phi) = 0 \tag{2.30}$$

The uniqueness of the solution implies that the linear operator $\mathcal{M}(t,\cdot) : L^2([0,t];\mathbb{R}^{2n}) \to L^2([0,t];\mathbb{R}^{2n})$, $t \neq t_{\alpha,\beta}$, is invertible. Now, we can come back to the general equation (2.24), written in the equivalent form:

$$\phi = \mathcal{M}^{-1}(t, \Psi_0(t,x,\eta) + \Psi_1(t,x,\phi)) \tag{2.31}$$

for all $t \neq t_{\alpha,\beta}$. By (2.26) and (2.27), we get the inequality

$$\|\phi\| \leq \|\mathcal{M}^{-1}(t,\cdot)\|_{L^2 \mapsto L^2}(C_0(T)\lambda(x,\eta) + C_1(T)) \leq K_1(t)\lambda(x,\eta) \tag{2.32}$$

where $K_1(t) := \|\mathcal{M}^{-1}(t,\cdot)\|_{L^2 \mapsto L^2}(C_0(T) + C_1(T))$. Finally, we have to prove the bound for the difference of any two solutions ϕ, ψ for the equation (2.31). In order to do this, we rewrite it under the form

$$\phi - \mathcal{M}^{-1}(t, \Psi_1(t,x,\phi)) = \mathcal{M}^{-1}(t, \Psi_0(t,x,\eta))$$

As a consequence,

$$\phi - \psi = \mathcal{M}^{-1}(t, \Psi_1(t,x,\phi)) - \mathcal{M}^{-1}(t, \Psi_1(t,x,\psi)).$$

Recalling (2.27) we have

$$\|\phi - \psi\|_{L^2} \leq \|\mathcal{M}^{-1}(t,)\|_{L^2 \mapsto L^2}\|\Psi_1(t,x,\phi) - \Psi_1(t,x,\psi)\|_{L^2} \leq \|\mathcal{M}^{-1}(t,)\|_{L^2 \mapsto L^2} 2C_1(T) =: E(t)$$

and this concludes the proof. □

2.3 Generating function with finitely many parameters

In this section we describe how the global parametrization of the graph Λ_t of the Hamiltonian flow can be actually obtained through a generating function with finitely many parameters. To this end we use the reduction of the Hamilton-Helmholtz functional due to Amann, Conley and Zehnder (see [AZ], [CZ], [Car], [B-C]). In this way we find, for the graph Λ_t of the Hamiltonian flow, a global parametrization of type:

$$\Lambda_t = \{(y,\eta;x,p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x S, \quad y = \nabla_\eta S, \quad 0 = \nabla_\theta S(t,x,\eta,\theta)\}$$

The essence of the Amann-Conley-Zehnder reduction is the existence of an underlying finite dimensional structure for the equation investigated in the previous section:

$$(\phi^x,\phi^p) = G_t(x,\eta,\phi^x,\phi^p) \qquad (\phi^x,\phi^p) \in L^2([0,T];\mathbb{R}^{2n}). \tag{2.33}$$

We can indeed consider the two orthogonal projectors

$$\mathbb{P}_M\phi(s) = \sum_{|r|\le M} \phi^{(r)} e_r(s) \qquad \mathbb{Q}_M\phi(s) = \sum_{|r|>M} \phi^{(r)} e_r(s)$$

generated by any orthonormal basis of $L^2([0,T];\mathbb{R}^{2n})$; for instance $e_r(s) := \frac{1}{\sqrt{T}} e^{\frac{2\pi}{T} irs} : r \in \mathbb{Z}$. Then, let us introduce the decomposition:

$$(f^x(\theta), f^p(\theta)) = \mathbb{Q}_M G_t\left(x,\eta,\theta^x + f^x(\theta),\theta^p + f^p(\theta)\right) \tag{2.34}$$

$$(\theta^x,\theta^p) = \mathbb{P}_M G_t\left(x,\eta,\theta^x + f^x(\theta),\theta^p + f^p(\theta)\right) \tag{2.35}$$

and prove the following

Lemma 2.10. *For $M \in \mathbb{N}$ large enough the functional equation (2.34) admits a unique solution $f(\theta) : \mathbb{P}_M L^2 \to \mathbb{Q}_M L^2$. The solutions of (2.33) can then be written in the form*

$$(\phi^x,\phi^p) = (\theta^x + f^x(\theta), \theta^p + f^p(\theta))$$

where $\theta \in \mathbb{P}_M L^2 \simeq \mathbb{R}^k$ are finite dimensional parameters solving the fixed point equation (2.35) on $\mathbb{R}^k$, $k = 2n(2M+1)$.

Proof. Let us first verify that, if $M \in \mathbb{N}$ is large enough, the equation (2.34) realizes in fact a contraction on $C^0(L^2,L^2)$. Hence it admits a unique solution $f(t,x,\theta) = (f^x(t,x,\theta), f^p(t,x,\theta))$. By (2.15), (2.16) the two equations read:

$$(f^x(t,x,\theta)(s), f^p(t,x,\theta)(s)) = \mathbb{Q}_M\left(\frac{1}{m}\int_0^s f^p(\theta)(\tau)\; d\tau, -\nabla V\left(x - \int_s^t \theta^x(\tau) + f^x(\theta)(\tau) d\tau\right)\right)$$

$$(\theta^x(s), \theta^p(s)) = \mathbb{P}_M\left(\frac{\eta}{m} + \frac{1}{m}\int_0^s \theta^p(\tau) + f^p(\theta)(\tau)\ d\tau, -\nabla V\left(x - \int_s^t \theta^x(\tau) + f^x(\theta)(\tau) d\tau\right)\right)$$

It is proved in [Car] (Lemma 6) that the contraction property holds if:

$$T^2 \sup_{(x,p)\in T^\star\mathbb{R}^n} |\nabla^2\mathcal{H}(x,p)|\ \frac{1+\sqrt{2M}}{2\pi M} < 1 \tag{2.36}$$

By Definition 2.4 it follows that $\sup_{(x,p)\in T^\star\mathbb{R}^n} |\nabla^2\mathcal{H}(x,p)| < +\infty$ and consequently given $0 < T < \infty$ we get the contraction property for the first equation choosing $M(T)$ large enough. In general, the second equation have many solutions depending on the values of (t, x). □

In this finite dimensional setting, we can consider the following set of curves, with $t \in [0, T]$:

$$\begin{cases} \gamma^x(t,x,\theta+f(\theta))(s) = x - \displaystyle\int_s^t \phi^x(t,x,\theta)(\tau)\ d\tau, & \phi^x(t,x,\theta) = \theta^x + f^x(t,x,\theta), \\ \gamma^p(t,x,\theta+f(\theta))(s) = \displaystyle\int_0^s \phi^p(t,x,\theta)(\tau)\ d\tau, & \phi^p(t,x,\theta) = \theta^p + f^p(t,x,\theta) \end{cases} \tag{2.37}$$

We note that this is a finite reduction of (2.4), but still contains all curves solving Hamilton's equations with boundary data $\gamma^x(t) = x$ and $\gamma^p(0) = 0$ because of ϕ are solving equation (2.33). Moreover, by a Sobolev's immersion theorem, $\Gamma \subset H^1([0,T]; T^\star\mathbb{R}^n) \subset C^0([0,T]; T^\star\mathbb{R}^n)$ and this entails their continuity.

We can now proceed to define the main object of this section:

Definition 2.11. *The finitely-many parameters generating function of Λ_t is defined as:*

$$\begin{aligned} S(t,x,\eta,\theta) &:= \langle x,\eta\rangle + \int_0^t \gamma^p(s)\dot\gamma^x(s) - H(\gamma^x(s), \eta+\gamma^p(s))\ ds\Big|_{\gamma(\cdot)=\gamma(t,x,\theta+f(t,x,\theta))(\cdot)} \\ &= \mathcal{S}(t,x,\eta,\theta+f(t,x,\theta)). \end{aligned} \tag{2.38}$$

Here $\mathcal{S}$ is the infinite dimensional generating function of Definition 2.3.

Remark The above generating function is fully parametrized by $\theta + f(t,x,\theta)$, $\theta \in \mathbb{R}^k$, and not by an arbitrary $\phi \in L^2$. This is the core of the finite reduction.

Now we provide a more detailed study about the analytical properties of f.

Lemma 2.12. *Consider the pair of functions (f^x, f^p). Then:*

(1) (f^x, f^p) *fulfill the following equations*

$$\begin{aligned}
f^x(s) &= \frac{1}{m}\mathbb{Q}_M \int_0^s \mathbb{Q}_M \int_\tau^t (L+L^\dagger) f^x(r)drd\tau + \Phi^x(t,x,\theta,f^x)(s) \\
f^p(s) &= \mathbb{Q}_M \int_s^t (L+L^\dagger) f^x(\tau)d\tau + \Phi^p(t,x,\theta,f^x)(s) \\
\Phi^x(t,x,\theta,f^x)(s) &:= -\frac{1}{m}\mathbb{Q}_M \int_0^s \mathbb{Q}_M \nabla V_0 \left(x - \int_\tau^t \theta^x(r) + f^x(r)dr \right) d\tau. \\
\Phi^p(t,x,\theta,f^x)(s) &:= -\mathbb{Q}_M \nabla V_0 \left(x - \int_s^t \theta^x(r) + f^x(r)dr \right) \qquad (2.39)
\end{aligned}$$

(2) Under the condition

$$d := \frac{T^2}{m}\|\mathbb{Q}_M\|^2 \|L+L^\dagger\| < 1, \qquad (2.40)$$

they fulfill the estimates:

$$\begin{aligned}
\|f^x(t,x,\theta)(\cdot)\|_{L^2} &\leq (1-d)^{-1}\frac{T^{\frac{3}{2}}}{m}\|\mathbb{Q}_M\|^2 \|\nabla V_0\|_{C^0} \\
\|f^p(t,x,\theta)(\cdot)\|_{L^2} &\leq T\|L\|\|\mathbb{Q}_M\|\|f^x(t,x,\theta)(\cdot)\|_{L^2} + \frac{T^{\frac{1}{2}}}{m}\|\mathbb{Q}_M\|\|\nabla V_0\|_{C^0} \qquad (2.41)
\end{aligned}$$

(3) If in addition

$$\frac{T^2}{m}\|\mathbb{Q}_M\|^2 \sup_{|i|+|j|\geq 2} \sup_{x,p} |\partial_x^i \partial_p^j \mathcal{H}(x,p)|^2 < 1 \qquad (2.42)$$

then there exist $C_{\alpha\sigma}(T) > 0$ *such that:*

$$\|\partial_x^\alpha \partial_\theta^\sigma f(t,x,\theta)(\cdot)\|_{L^2} \leq C_{\alpha\sigma}(T) \qquad (2.43)$$

Proof. By direct computation, the first functional equation reads:

$$\begin{aligned}
f^x(s) &= \frac{1}{m}\mathbb{Q}_M \int_0^s f^p(\theta)(\tau)\, d\tau \\
&= \frac{1}{m}\mathbb{Q}_M \int_0^s -\mathbb{Q}_M \nabla V \left(x - \int_\tau^t \theta^x(r) + f^x(r)dr \right) \, d\tau \\
&= -\frac{1}{m}\mathbb{Q}_M \int_0^s \mathbb{Q}_M (L+L^\dagger) \left(x - \int_\tau^t \theta^x(r) + f^x(r)dr \right) d\tau \\
&- \frac{1}{m}\mathbb{Q}_M \int_0^s \mathbb{Q}_M \nabla V_0 \left(x - \int_\tau^t \theta^x(r) + f^x(r)dr \right) d\tau \\
&= \frac{1}{m}\mathbb{Q}_M \int_0^s \mathbb{Q}_M \int_\tau^t (L+L^\dagger) f^x(r)drd\tau + \Phi^x(t,x,\theta,f^x)(s)
\end{aligned}$$

where the last equality follows by (2.39). Analogous computation for $f^p(s)$:

$$f^p(t,x,\theta)(s) = \mathbb{Q}_M \int_s^t (L+L^\dagger) f^x(\tau)d\tau + \Phi^p(t,x,\theta,f^x)(s)$$

This proves Assertion (1).

To see Assertion (2), remark that (2.39) also entails:

$$\|\Phi^x(t,x,\theta,f^x)(\cdot)\|_{L^2} \leq \frac{T^{\frac{3}{2}}}{m}\|\mathbb{Q}_M\|^2\|\nabla V_0\|_{C^0} \tag{2.44}$$

whence we obtain:

$$\|f^x(t,x,\theta)(\cdot)\|_{L^2} \quad \leq \quad \frac{T^2}{m}\|\mathbb{Q}_M\|^2\|L+L^\dagger\|\|f^x(t,x,\theta)(\cdot)\|_{L^2} + \|\Phi(t,x,\eta,\theta)(\cdot)\|_{L^2}$$

If we choose M large enough, then $d := \frac{T^2}{m}\|\mathbb{Q}_M\|^2\|L+L^\dagger\| < 1$ and hence we get

$$\|f^x(t,x,\theta)(\cdot)\|_{L^2} \quad \leq \quad (1-d)^{-1}\frac{T^{\frac{3}{2}}}{m}\|\mathbb{Q}_M\|^2\|\nabla V_0\|_{C^0}$$

In the same way we have the estimate:

$$\begin{aligned}\|f^p(t,x,\theta)(\cdot)\|_{L^2} &\leq T^{\frac{1}{2}}\|L+L^\dagger\|\|\mathbb{Q}_M\|\|f^x(t,x,\theta)(\cdot)\|_{L^2} + \|\Phi^p(t,x,\eta,\theta)(\cdot)\|_{L^2} \\ &\leq T^{\frac{1}{2}}\|L+L^\dagger\|\|\mathbb{Q}_M\|\|f^x(t,x,\theta)(\cdot)\|_{L^2} + T^{\frac{1}{2}}\|\mathbb{Q}_M\|\|\nabla V_0\|_{C^0}\end{aligned}$$

This proves Assertion (2).

The equation for the first order partial derivatives reads:

$$\begin{aligned}\frac{\partial f^{x,\alpha}}{\partial x_i}(t,x,\theta) &= \frac{\mathbb{Q}_M}{m}\int_0^s \mathbb{Q}_M\int_\tau^t (L+L^\dagger)\frac{\partial f^{x,\alpha}}{\partial x_i}(t,x,\theta)(r)drd\tau \\ &+ \frac{\mathbb{Q}_M}{m}\int_0^s \mathbb{Q}_M\frac{\partial^2 V_0}{\partial x_\alpha \partial x_\beta}\left(x - \int_\tau^t \theta^x(r) + f^x(t,x,\theta)(r)dr\right)\left(\delta_{\beta i} + \int_\tau^t \frac{\partial f^{x,\beta}}{\partial x_i}(t,x,\theta)(r)dr\right)d\tau\end{aligned}$$

If M is large enough, then $d' := \frac{T^2}{m}\|\mathbb{Q}_M\|^2\|L+L^\dagger\| + \frac{T^2}{m}\|\mathbb{Q}_M\|^2\|\nabla^2 V_0\|_{C^0} < 1$ and we get:

$$\left\|\frac{\partial f^x}{\partial x_i}(t,x,\theta)(\cdot)\right\|_{L^2} < (1-d')^{-1}\frac{T^{\frac{3}{2}}}{m}\|\mathbb{Q}_M\|^2\|\nabla^2 V_0\|_{C^0}$$

The equation for the second order partial derivatives reads:

$$\begin{aligned}\frac{\partial^2 f^{x,\alpha}}{\partial x_i \partial x_j}(t,x,\theta) &= \frac{\mathbb{Q}_M}{m}\int_0^s \mathbb{Q}_M\int_\tau^t (L+L^\dagger)\frac{\partial^2 f^{x,\alpha}}{\partial x_i \partial x_j}(t,x,\theta)(r)drd\tau \\ &+ \frac{\mathbb{Q}_M}{m}\int_0^s \mathbb{Q}_M\frac{\partial^2 V_0}{\partial x_\alpha \partial x_\beta}\left(x - \int_\tau^t \theta^x(r) + f^x(t,x,\theta)(r)dr\right)\left(\int_\tau^t \frac{\partial^2 f^{x,\beta}}{\partial x_i \partial x_j}(t,x,\theta)(r)dr\right)d\tau \\ &+ \frac{\mathbb{Q}_M}{m}\int_0^s \mathbb{Q}_M F_{\alpha\beta k}(t,x,\theta)(\tau)\left(\delta_{kj} + \int_\tau^t \frac{\partial f^{x,k}}{\partial x_j}(t,x,\theta)(r)dr\right)\left(\delta_{\beta i} + \int_\tau^t \frac{\partial f^{x,\beta}}{\partial x_i}(t,x,\theta)(r)dr\right)d\tau\end{aligned}$$

where

$$F_{\alpha\beta k}(t,x,\theta)(\tau) := \frac{\partial^3 V_0}{\partial x_\alpha \partial x_\beta \partial x_k}\left(x - \int_\tau^t \theta^x(r) + f^x(t,x,\theta)(r)dr\right)$$

As before, if we require $d'' := \frac{T^2}{m}\|\mathbb{Q}_M\|^2(\|L+L^\dagger\| + \|\nabla^2 V_0\|_{C^0} + \|F\|_{C^0}) < 1$ then

$$\left\| \frac{\partial^2 f^x}{\partial x_i \partial x_j}(t,x,\theta)(\cdot) \right\|_{L^2} < (1-d'')^{-1}\frac{1}{m}\|\mathbb{Q}_M\|^2\|F\|_{C^0}\left(T^{\frac{3}{2}} + T^4\|\nabla f^x\|^2_{L^2} + 2T^2\|\nabla f^x\|_{L^2}\right)$$

For the higher order derivatives in x and also for θ-partial derivatives we can proceed in the same way, with the general condition

$$\frac{T^2}{m}\|\mathbb{Q}_M\|^2 \sup_{|i|+|j|\geq 2}\sup_{x,p}|\partial_x^i\partial_p^j\mathcal{H}(x,p)|^2 < 1 \tag{2.45}$$

in order to conclude the existence of $C_{\alpha\sigma}(T) > 0$ such that

$$\|\partial_x^\alpha\partial_\theta^\sigma f(t,x,\theta)(\cdot)\|_{L^2} \leq C_{\alpha\sigma}(T). \tag{2.46}$$

This proves Assertion (3) and thus concludes the proof of the Lemma. □

Theorem 2.13. *The generating function (2.38) admits the following representation:*

$$\begin{aligned} S &= \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle Q(t)\theta,\theta\rangle + \langle v(t,x,\eta),\theta + f(t,x,\theta)\rangle + \langle \nu(t,x,\theta),\theta\rangle \\ &+ g(t,x,\theta). \end{aligned} \tag{2.47}$$

Here: $\theta \in \mathbb{R}^k$; $t \mapsto Q(t) \in GL(n)$, $Q(0) = 0$; more overthere are $C_{\alpha\beta\sigma}(T) > 0$ such that

$$|\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma g| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma \nu| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma f| \leq C_{\alpha\beta\sigma}(T).$$

The function $(t,x,\eta) \mapsto v(t,x,\eta)$ is linear in x,η, and finally:

$$k > CT^4 \sup_{|\alpha|+|\beta|\geq 2}\sup_{x,p}|\partial_x^\alpha\partial_p^\beta\mathcal{H}(x,p)|^2. \tag{2.48}$$

Proof. By the explicit upper bound $\|\mathbb{Q}_M\| \leq \dfrac{T}{2\pi}\sqrt{\dfrac{2}{M}}$ of (2.42) we have

$$k > CT^4 \sup_{|\alpha|+|\beta|\geq 2}\sup_{x,p}|\partial_x^\alpha\partial_p^\beta\mathcal{H}(x,p)|^2.$$

We recall the structure of the infinite dimensional generating function:

$$\mathcal{S}(t,x,\eta,\phi) = \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle R(t)\phi,\phi\rangle + \langle v(t,x,\eta),\phi\rangle + \sigma(t,x,\phi)$$

As a consequence:

$$\begin{aligned} S(t,x,\eta,\theta) &:= \mathcal{S}(t,x,\eta,\theta + f(t,x,\theta)) \\ &= \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle R(t)(\theta + f(t,x,\theta)),\theta + f(t,x,\theta)\rangle \\ &+ \langle v(t,x,\eta),\theta + f(t,x,\theta)\rangle + \sigma(t,x,\theta + f(t,x,\theta)). \end{aligned}$$

We can thus make the identifications:

$$\begin{aligned}\langle Q(t)\theta,\theta\rangle &:= \langle R(t)\theta,\theta\rangle\\ \langle \nu(t,x,\theta),\theta\rangle &:= \langle 2R(t)f(t,x,\theta),\theta\rangle\\ g(t,x,\theta) &:= \sigma(t,x,\theta+f(t,x,\theta))+\langle R(t)f(t,x,\theta),f(t,x,\theta)\rangle \end{aligned}\tag{2.49}$$

Now it is easy to see that

$$|\nu(t,x,\theta)|\leq 2\|R(t)\|\|f(t,x,\theta)(\cdot)\|_{L^2}\leq C(T)$$

and this entails boundedness with respect to the θ-variables. Moreover the same property holds true for the other term. We have indeed:

$$|g(t,x,\theta)|\leq \|\sigma(t,x,\phi)(\cdot)\|_{C^0}+\|R(t)\|\|f(t,x,\theta)(\cdot)\|^2_{L^2}\leq C'(T)$$

By using the above results we then get the existence of $C'(T)$ such that $|g(t,x,\theta)\leq C'(T)$. The estimates for the partial derivatives follow in the same way. □

Theorem 2.14. *The graph of the Hamiltonian flow*

$$\Lambda_t:=\left\{(y,\eta;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n \mid (x,p)=\phi^t_{\mathcal{H}}(y,\eta)\right\}$$

admits a global generating function with finitely many parameters:

$$\Lambda_t=\{(y,\eta;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n \mid p=\nabla_x S,\quad y=\nabla_\eta S,\quad 0=\nabla_\theta S(t,x,\eta,\theta)\}$$

Proof. By Proposition (2.6) we can write:

$$\Lambda_t=\left\{(y,\eta;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n \mid p=\nabla_x\mathcal{S},\quad y=\nabla_\eta\mathcal{S},\quad 0=\frac{D\mathcal{S}}{D\phi}\right\}$$

where $\mathcal{S}$ is the infinite-dimensional generating function of Definition 2.3. Now we remark that the finite-dimensional stationarity condition:

$$0=\nabla_\theta S(t,x,\eta,\theta^\star)$$

is equivalent to the variational equation expressing the stationarity:

$$0=\frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi^\star)$$

Indeed, by Lemma 2.10 and [Car] (see Lemma 7), there is a bijective correspondence between the solutions of the two equations, $\phi^\star=\theta^\star+f(t,x,\theta^\star)$. Moreover it is easy to prove that

$$\nabla_x S|_{(t,x,\eta,\theta^\star)}=\nabla_x\mathcal{S}|_{(t,x,\eta,\phi^\star)},\qquad \nabla_\eta S|_{(t,x,\eta,\theta^\star)}=\nabla_\eta\mathcal{S}|_{(t,x,\eta,\phi^\star)}$$

This is true because of the definition $S(t,x,\eta,\theta) := \mathcal{S}(t,x,\eta,\theta+f(t,x,\theta))$, and the computation

$$\nabla_x S(t,x,\eta,\theta) = \nabla_x \mathcal{S}(t,x,\eta,\phi)|_{\phi=\theta+f(t,x,\theta)} + \frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi)|_{\phi=\theta+f(t,x,\theta)}[\nabla_x f(t,x,\theta)].$$

Evaluating both sides on the solutions $\theta^\star$ we get the relation. The same argument applies to $\nabla_\eta S$, and this concludes the proof. □

Theorem 2.15. *The Hamilton-Jacobi equation is solved by the smooth function $S(t,x,\eta,\theta)$ on the stationary points $\Sigma_S = \{(x,\eta,\theta) \in R^{2n+k} \mid \nabla_\theta S(t,x,\eta,\theta) = 0\}$. More precisely:*

$$\begin{cases} \partial_t S(t,x,\eta,\theta) + \dfrac{|\nabla_x S|^2}{2m}(t,x,\eta,\theta) + V(x) = 0, \\ S(0,x,\eta,\theta) = \langle x,\eta\rangle; \quad (x,\eta,\theta) \in \Sigma_S. \end{cases} \tag{2.50}$$

Proof. We recall that, by Proposition 2.7, the Hamilton-Jacobi equation is solved by $\mathcal{S}(t,x,\eta,\phi)$ on the infinite dimensional stationary points defined by $\dfrac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi^\star) = 0$.

$$\begin{cases} \partial_t \mathcal{S}(t,x,\eta,\phi) + \dfrac{|\nabla_x \mathcal{S}|^2}{2m}(t,x,\eta,\phi) + V(x) = 0, \quad (t,x) \in \mathbb{R}\times\mathbb{R}^n \\ \mathcal{S}(0,x,\eta,\phi) = \langle x.\eta\rangle, \quad \dfrac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi) = 0. \end{cases} \tag{2.51}$$

On the other hand, we have

$$\nabla_x S|_{(t,x,\eta,\theta^\star)} = \nabla_x \mathcal{S}|_{(t,x,\eta,\phi^\star)}, \qquad \partial_t S|_{(t,x,\eta,\theta^\star)} = \partial_t \mathcal{S}|_{(t,x,\eta,\phi^\star)} \tag{2.52}$$

Indeed the first equality is proved in the previous theorem; whereas for the second one we observe:

$$\partial_t S(t,x,\eta,\theta) = \partial_t \mathcal{S}(t,x,\eta,\phi)|_{\phi=\theta+f(t,x,\theta)} + \frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi)|_{\phi=\theta+f(t,x,\theta)}[\partial_t f(t,x,\theta)].$$

Since $\dfrac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi^\star) = 0$ the second equality in (2.52) is proved. (2.51) and (2.52) then yield the assertion. □

Theorem 2.16. *Let S and Σ_S be as in Theorem 2.15. Then there exists $\Theta_N \in C_b^\infty([0,T]\times \mathbb{R}^{2n+k};\mathbb{R})$ with $\Theta_N|_{\Sigma_S} = 0$, such that an equivalent generating function S_N is given by the solution of the problem*

$$\begin{cases} \dfrac{|\nabla_x S_N|^2}{2m}(t,x,\eta,\theta) + V(x) + \partial_t S_N(t,x,\eta,\theta) = \Theta_N, \\ S_N(0,x,\eta,\theta) = \langle x,\eta\rangle. \end{cases} \tag{2.53}$$

Moreover, defining:

$$\Pi(\Theta_N) := \mathrm{div}_\theta \left(\Theta_N \frac{\nabla_\theta S_N}{|\nabla_\theta S_N|^2} \right) \tag{2.54}$$

S_N enjoys the property:

$$\Pi^j(\Theta_N) \in C_b^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R}) \qquad \forall 1 \le j \le N, \quad N = 1, 2, \dots \tag{2.55}$$

Proof. We remember that $\Sigma_S \subset \mathbb{R}^{2n+k}$ is a submanifold of dimension $2n$ thanks to the nondegeneracy condition

$$rk(\nabla^2_{x\theta} S, \nabla^2_{\eta\theta} S, \nabla^2_{\theta\theta} S)|_{\Sigma_S} = max = k = 2n(2N+1)$$

for some $N \ge 1$. We define $z := (x, \eta, \theta) \in \mathbb{R}^{2n+k}$ and for any point $\bar{z} \in \Sigma_S$. Define furthermore $\widetilde{S}$ (not necessarily uniquely) through the conditions:

$$\partial_t \widetilde{S}(t,z) = \partial_t S(t,\bar{z}) + L(t,z), \tag{2.56}$$

$$\nabla_z \widetilde{S}(t,z) = \nabla_z S(t,\bar{z}) + F(t,z), \tag{2.57}$$

$$\Delta_x \widetilde{S}(t,z) = \Delta_x S(t,\bar{z}) + G(t,z), \tag{2.58}$$

where $L = (L^x, L^\eta, L^\theta) \in C_b^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R})$ and $L(t,\bar{z}) = 0$, the perturbation of the gradient in (2.57) is $F = (F^x, F^\eta, F^\theta) \in C_b^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R}^{2n+k})$ with $F(t,\bar{z}) = 0$ while in (2.63) we require $G \in C_b^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R})$ and $G(t,\bar{z}) = 0$. In addition, we require that $F^\theta(t,z) \neq 0$ for $z \notin \Sigma_S$. Hence the new stationarity equation:

$$\nabla_\theta \widetilde{S}(t,z) = F^\theta(t,z) \tag{2.59}$$

implies $\Sigma_{\widetilde{S}} = \Sigma_S$. In order to verify (2.54) we require a suitable asymptotic behaviour of L, F, G around Σ_S. Indeed,

$$\partial_t \widetilde{S}(t,z) = \partial_t S(t,\bar{z}) + L(t,z), \qquad \nabla_x \widetilde{S}(t,z) = \nabla_x S(t,\bar{z}) + F^x(t,z).$$

So, by easy computations and by (2.50), we have

$$\begin{aligned}
\Theta(t,z) &= \frac{|\nabla_x \widetilde{S}|^2}{2m}(t,z) + V(x) + \partial_t \widetilde{S}(t,z) \\
&= \frac{1}{2m} |\nabla_x S(t,\bar{z}) + F^x(t,z)|^2 + V(x) + \partial_t S(t,\bar{z}) + L(t,z) \\
&= \frac{1}{2m} |\nabla_x S(t,\bar{z})|^2 + V(x) + \partial_t S(t,\bar{z}) + \frac{1}{m} \nabla_x S(t,\bar{z}) F^x(t,z) + \frac{1}{2m} |F^x(t,z)|^2 + L(t,z) \\
&= \frac{1}{m} \nabla_x S(t,\bar{z}) F^x(t,z) + \frac{1}{2m} |F^x(t,z)|^2 + L(t,z)
\end{aligned} \tag{2.60}$$

Now we can always require that the vanishing asymptotic behaviour of F^x, F^θ, L around Σ_S are such that it holds:

$$\Pi(\Theta) := \operatorname{div}\left(\Theta \frac{\nabla_\theta \widetilde{S}}{|\nabla_\theta \widetilde{S}|^2}\right) \in C_b^\infty([0,T]\times\mathbb{R}^{2n+k};\mathbb{R})$$

By the same arguments as above, we can look for S_N such that $\Sigma_{S_N} = \Sigma_S$ and

$$\partial_t S_N(t,z) = \partial_t S(t,\bar{z}) + L_N(t,z), \tag{2.61}$$

$$\nabla_z S_N(t,z) = \nabla_z S(t,\bar{z}) + F_N(t,z), \tag{2.62}$$

$$\Delta_x S_N(t,z) = \Delta_x S(t,\bar{z}) + G_N(t,z), \tag{2.63}$$

where F_N^x, F_N^θ and L_N are chosen in such a way that:

$$\Pi^j(\Theta_N) \in C_b^\infty([0,T]\times\mathbb{R}^{2n+k};\mathbb{R}) \qquad \forall 1 \le j \le N$$

□

Let us examine the topology of the finite-dimensional critical points set.

Theorem 2.17. *Let S be as in Definition 2.11, and $\lambda(x,\eta)$, $t_{\alpha,\beta}$ as in (2.19) and (2.20), respectively. Consider $(t,x,\eta) \in]0,T] \times \mathbb{R}^n \times \mathbb{R}^n$. Then:*
(1) All solutions $\theta \in \mathbb{P}_M L^2([0,T];\mathbb{R}^{2n}) \simeq \mathbb{R}^k$ of the stationarity equation:

$$0 = \nabla_\theta S(t,x,\eta,\theta)$$

fulfill the estimates

$$\|\theta\|_{L^2} > \tilde{K}_2(T)\lambda(x,\eta) \quad \forall t \in]0,T], \qquad |x|^2+|\eta|^2 > D(T)^2; \tag{2.64}$$

$$\|\theta\|_{L^2} \le \tilde{K}_1(t)\lambda(x,\eta) \quad \forall t \ne t_{\alpha,\beta}, \quad \forall (x,\eta) \in \mathbb{R}^{2n}. \tag{2.65}$$

where $D(T) < +\infty$, $\tilde{K}_2(T) < +\infty$ while $\tilde{K}_1(t) < +\infty$ is a constant defined for $t \ne t_{\alpha,\beta}$.
(2) The difference of any two solutions θ, ω fulfills the inequality

$$\|\theta - \omega\|_{L^2} \le \tilde{E}(t) \quad \forall t \ne t_{\alpha,\beta}, \quad \forall (x,\eta) \in \mathbb{R}^{2n}. \tag{2.66}$$

Proof. By Proposition 2.9 and Lemma 2.10 all solutions $\phi \in L^2$of the variational equation

$$0 = \frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi)$$

are such that

$$\phi = \theta + f(t,x,\theta)$$

and fulfill the inequalities (2.21), (2.22) and (2.23) for some constants $K_1(t), K_2(T)$ and $E(t)$. Using the uniform bound proved in Lemma 2.12:

$$\|f(t,x,\theta)(\cdot)\|_{L^2} \leq C_{00}(T)$$

we easily establish the existence of the new constants $\tilde{K}_1(t)$, $\tilde{K}_2(T)$ and $\tilde{E}(t)$. □

Theorem 2.18. *Let us suppose* $V(x) = \frac{1}{2}|x|^2 + V_0(x)$ *with* $\sup_{x\in\mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1$, $(t,x,\eta) \in]0,T] \times \mathbb{R}^{2n}$ *and* $t \neq (2\tau+1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$. *Then the following quadratic form:*

$$\langle \nabla^2_\theta S(t,x,\eta,\theta)u, u\rangle, \qquad u \in \mathbb{R}^k,$$

is non degenerate on all points solving $\nabla_\theta S(t,x,\eta,\theta) = 0$.

Proof. The quadratic form is non degenerate if and only if the solutions θ of the equation

$$\nabla_\theta S(t,x,\eta,\theta) = 0 \tag{2.67}$$

are isolated points. This property can be translated in the infinite dimensional setting of the equation

$$\frac{D\mathcal{S}}{D\phi}(t,x,\eta,\phi) = 0$$

thanks to the equivalence $\phi = \theta + f(t,x,\theta)$ shown in Lemma 2.10. We recall that

$$\mathcal{S} = \langle x,\eta\rangle + \int_0^t \langle \int_0^s \phi^p(\tau)d\tau, \phi^x(s)\rangle - \frac{1}{2m}\left(\eta + \int_0^s \phi^p(\tau)d\tau\right)^2 - V\left(x - \int_s^t \phi^x(\tau)d\tau\right) ds$$

Now we perform the partial reduction of the infinite dimesional parameters, by means of the first stationarity equation $\frac{D\mathcal{S}}{D\phi^x}(t,x,\eta,\phi) = 0$ corresponding to $m\phi^x(s) = \eta + \int_0^s \phi^p(\tau)d\tau$ (essentially, the Legendre transform). Therefore we get the new functional:

$$\widetilde{\mathcal{S}}(t,x,\eta,\phi^x) = \langle x - \int_0^t \phi^x(\tau)d\tau, \eta\rangle + \int_0^t \frac{m}{2}\left[|\phi^x(s)|^2 - V\left(x - \int_s^t \phi^x(\tau)d\tau\right)\right] ds$$

Setting $\gamma^x(s) = x - \int_s^t \phi^x(\tau)d\tau$, we can consider the equivalent form

$$\mathcal{A}[\gamma^x] = \langle \gamma^x(0), \eta\rangle + \int_0^t \frac{m}{2}\left[|\dot\gamma^x(s)|^2 - V(\gamma^x(s))\right] ds$$

with the boundary conditions: $\gamma^x(t) = x$ and $m\dot\gamma^x(0) = \eta$. The second variation is:

$$\frac{D^2\mathcal{A}}{D\gamma}(\gamma^x)[\delta\gamma, \delta\dot\gamma] = \frac{1}{2}\int_0^t m\left[|\delta\dot\gamma(s)|^2 - \nabla^2 V(\gamma^x(s))\delta\gamma(s)\delta\gamma(s)\right] ds$$

Writing down the integrand under the form

$$\begin{pmatrix}\delta\gamma(s) \ \delta\dot{\gamma}(s)\end{pmatrix} \begin{pmatrix} -\nabla^2 V(\gamma^x(s)) & 0 \\ 0 & mI \end{pmatrix} \begin{pmatrix} \delta\gamma(s) \\ \delta\dot{\gamma}(s) \end{pmatrix}$$

we realize that requiring $\nabla^2 V(x)$ non-degenerate $\forall\, x \in \mathbb{R}^n$, then the second variation is a bilinear non degenerate functional. This implies that all the stationary curves of the action functional, namely the curves solving

$$\frac{D\mathcal{A}}{D\gamma}(\gamma^x)[v] = 0 \quad \forall v \in T\Gamma$$

are isolated points belonging to $H^1([0,t];\mathbb{R}^n)$. We conclude that the same property must hold for the points $\theta \in \mathbb{R}^k$ solving equation (2.67). □

Next, we investigate the number of solutions of the stationarity equation.

Theorem 2.19. *Let us suppose* $V(x) = \frac{1}{2}|x|^2 + V_0(x)$ *with* $\sup_{x\in\mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1$, $(t,x,\eta) \in]0,T] \times \mathbb{R}^{2n}$ *and* $t \neq (2\tau+1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$. *Then the stationarity equation*

$$\nabla_\theta S(t,x,\eta,\theta) = 0$$

has a finite number of solutions $\theta^\star_\alpha(t,x,\eta)$, $1 \le \alpha \le \mathcal{N}(t)$. *The upper bound has the expression:*

$$\mathcal{N}(t) \le \frac{(2\tilde{E}(t))^k}{\varepsilon(T)^k} \tag{2.68}$$

Here $\tilde{E}(t)$ *as in Theorem 2.17 whereas*

$$\varepsilon(T) := \frac{1}{k} \frac{\inf_{(t,x,\eta,\theta)} \sup_{i,j} \left|\frac{\partial^2 S}{\partial\theta_i \partial\theta_j}\right| (t,x,\eta,\theta)}{\sup_{(t,x,\eta,\theta)} \ \sup_{i,j,m} \left|\frac{\partial^3 S}{\partial\theta_i\partial\theta_j\partial\theta_m}\right| (t,x,\eta,\theta) + 1}. \tag{2.69}$$

Proof. By Theorem (2.17) all critical parameters must be contained in the compact set $\overline{B}_r \subset \mathbb{R}^k$ with $r := 2\tilde{E}(t)$. As a consequence, there exists a subsequence $\{\theta_{\alpha(j)}\}_{j\in\mathbb{N}}$ converging to some point $\bar{\theta}$ in $\overline{B}_r(0)$. However the function $\nabla_\theta S(t,x,\eta,\cdot)$ is continuous on $\mathbb{R}^k$. Hence the limit is also a critical point, namely $0 = \nabla_\theta S(t,x,\eta,\bar{\theta})$. By the previous theorem all the critical points of S are isolated. This is a contradiction, so their number must be finite. In order to obtain an upper bound for this number, we first observe that

$$\begin{aligned} \nabla^2_\theta S(t,x,\eta,\theta) &= \nabla^2_\theta S(t,x,\eta,\theta^\star) + \int_0^1 \frac{d}{d\lambda} \nabla^2_\theta S(t,x,\eta,\theta^\star + \lambda(\theta-\theta^\star))\, d\lambda \\ &= \nabla^2_\theta S(t,x,\eta,\theta^\star) + \int_0^1 D_\theta \nabla^2_\theta S(t,x,\eta,\theta^\star + \lambda(\theta-\theta^\star))\, d\lambda\ (\theta-\theta^\star) \end{aligned}$$

We know that, thanks to Theorem 2.18, the first matrix on the righthand side is non degenerate. In order to verify that the addition of the second one does not change this property, we establish the matrix norm inequality:

$$\left\| \int_0^1 D_\theta \nabla^2_\theta S(t,x,\eta,\theta^\star + \lambda(\theta - \theta^\star))\ d\lambda\ (\theta - \theta^\star) \right\|_2 < \|\nabla^2_\theta S(t,x,\eta,\theta^\star)\|_2. \tag{2.70}$$

Here $\|\cdot\|_2$ is the usual norm for the matrix viewed as an operator. Now denote $\varepsilon := \|\theta - \theta^\star\|$. The above inequality is a fortiori verified if:

$$\varepsilon\ \sqrt{k} \sup_{(t,x,\eta,\theta)} \sup_{i,j,m} \left| \frac{\partial^3 S}{\partial\theta_i \partial\theta_j \partial\theta_m} \right| (t,x,\eta,\theta) < \frac{1}{\sqrt{k}} \inf_{(t,x,\eta,\theta)} \sup_{i,j} \left| \frac{\partial^2 S}{\partial\theta_i \partial\theta_j} \right| (t,x,\eta,\theta) \tag{2.71}$$

because the l.h.s is an upper bound for the l.h.s. of (2.70) and the r.h.s a lower bound for the r.h.s. of (2.70). (2.71) is in turn a fortiori verified if:

$$\varepsilon\ \sqrt{k} \left(\sup_{(t,x,\eta,\theta)} \sup_{i,j,m} \left| \frac{\partial^3 S}{\partial\theta_i \partial\theta_j \partial\theta_m} \right| (t,x,\eta,\theta) + 1 \right) < \frac{1}{\sqrt{k}} \inf_{(t,x,\eta,\theta)} \sup_{i,j} \left| \frac{\partial^2 S}{\partial\theta_i \partial\theta_j} \right| (t,x,\eta,\theta) \tag{2.72}$$

and this yields (2.69). In this way, we have found the radius $\varepsilon(T)$ of the balls in $\mathbb{R}^k$, where each $\theta^\star$ is a unique local critical point. This local confinement of critical points together with the global one proved in Th 2.17, allows us to get an estimate of their total number N. We simply compute the ratio between the volume of the ball B_r containing all the points and the volume of the small isolating balls.

$$\mathcal{N}(t) = \frac{vol(B_r)}{vol(B_\varepsilon)} = \frac{(2\tilde{E}(t))^k}{\varepsilon(T)^k}$$

□

We use Theorem 2.19 in order to study the global behaviour of the stationarity equation.

Theorem 2.20. *Let us suppose* $V(x) = \frac{1}{2}|x|^2 + V_0(x)$ *with* $\sup_{x\in\mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1$, $(t,x,\eta) \in]0,T] \times \mathbb{R}^{2n}$ *and* $t \neq (2\tau+1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$. *Let the number* $\mathcal{N}(t)$ *be given by (2.68). Then there exists a finite open partition* $\mathbb{R}^{2n} = \bigcup_{\ell=1}^{\mathcal{N}(t)} D_\ell$ *such that the equation*

$$0 = \nabla_\theta S(t,x,\eta,\theta) \tag{2.73}$$

admits on each D_ℓ *exactly* ℓ *smooth solutions* $\theta^\star_\alpha(t,x,\eta)$, $1 \leq \alpha \leq \ell$.

Proof. We recall that $\Sigma_S := \{(x,\eta,\theta) \in \mathbb{R}^{2n+k} |\ 0 = \nabla_\theta S(t,x,\eta,\theta)\}$ is a $2n$-dimensional submanifold of $\mathbb{R}^{2n+k}$ diffeomorphic to Λ_t. Moreover, by the nondegeneracy hypothesis on

$\nabla^2 V$ we have the transversal behaviour of Σ_S (with respect to $(x,\eta) \in \mathbb{R}^{2n}$) almost everywhere; namely the rank of $\nabla^2_\theta S$ can differ from its maximum value (k) only on subsets whose projection on $(x,\eta) \in \mathbb{R}^{2n}$ is of zero measure. The condition of transversality is fulfilled on components D_ℓ (locally diffeomorphic to open sets of $\mathbb{R}^{2n}$) where the local smooth inversion of equation (2.73) is possible, yielding ℓ functions $\theta^\star_\alpha(t,x,\eta)$. This argument works up to the finite maximum value $\mathcal{N}(t)$. □

2.4 Transport equations

We conclude this section by introducing transport equations in a global geometrical setting.

Theorem 2.21. *Let us consider $\rho \in \mathcal{S}(\mathbb{R}^k;\mathbb{R})$ with $\|\rho\|_{L^1} = 1$. The transport equation written on the stationary points Σ_S of the generating function S,*

$$\begin{cases} \partial_t b_0 + \frac{1}{m}\nabla_x S\ \nabla_x b_0 + \frac{1}{2m}\Delta_x S\ b_0(t,x,\eta,\theta) = 0, \\ \\ b_0(0,x,\eta,\theta) = \rho(\theta), \quad (x,\eta,\theta) \in \Sigma_S. \end{cases} \tag{2.74}$$

admits the following solution:

$$b_0(t,x,\eta,\theta) = \exp\left\{-\frac{1}{2m}\int_0^t \Delta_x S(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)d\tau\right\}\rho(\theta) \tag{2.75}$$

where γ^x is the family of curves defined in (2.37).

Proof. The inital condition is immediately verified:

$$b_0(0,x,\eta,\theta) = \rho(\theta)$$

Recalling the results of Proposition 2.6 and Theorem 2.14, we compute the expression of the differential operator $\partial_t b_0 + \frac{1}{m}\nabla_x S\ \nabla_x b_0(t,x,\eta,\theta)$ when evaluated on the submanifold $\Sigma_S := \{(x,\eta,\theta) \in \mathbb{R}^{2n+k} \mid 0 = \nabla_\theta S(t,x,\eta,\theta)\}$. Namely,

$$\begin{aligned} \partial_t b_0 + \frac{1}{m}\nabla_x S\ \nabla_x b_0(t,x,\eta,\theta)\Big|_{\Sigma_S} &= \partial_t b_0 + \frac{1}{m}\left(\eta + \gamma^p(t,x,\theta)(t)\right)\nabla_x b_0(t,x,\eta,\theta)\Big|_{\Sigma_S} \\ &= \partial_t b_0 + \dot\gamma^x(t,x,\theta)(t)\nabla_x b_0(t,x,\eta,\theta)\Big|_{\Sigma_S} \\ &= \partial_\mu b_0(\mu,x,\eta,\theta) + \dot\gamma^x(t,x,\theta)(\mu)\nabla_x b_0(\mu,x,\eta,\theta)\Big|_{\Sigma_S}\Big|_{\mu=t} \\ &= \frac{d}{d\mu} b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta)\Big|_{\Sigma_S}\Big|_{\mu=t} \end{aligned} \tag{2.76}$$

where the expression of $\frac{1}{2m}\Delta_x S(t,x,\eta,\theta)\ b_0(t,x,\eta,\theta)$ is:

$$\frac{1}{2m}\Delta_x S(t,x,\eta,\theta)\ b_0(t,x,\eta,\theta) = \frac{1}{2m}\Delta_x S(t,\gamma^x(t,x,\theta)(\mu),\eta,\theta)\ b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta)\Big|_{\mu=t}$$

Now, we write down the equation in the new variable μ and for all $(x,\eta,\theta)\in\mathbb{R}^{2n+k}$:

$$\frac{d}{d\mu}b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta) + \frac{1}{2}\Delta_x S(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta)\ b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta) = 0$$

If we define $\alpha(\mu) := b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta)$ we can rewrite the previous equation as

$$\frac{d}{d\mu}\alpha(\mu) = -\frac{1}{2m}\Delta_x S(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta)\ \alpha(\mu).$$

where the variables (t,x,η,θ) have to be considered as fixed. This yields:

$$b_0(\mu,\gamma^x(t,x,\theta)(\mu),\eta,\theta) = \exp\left\{-\frac{1}{2m}\int_0^\mu \Delta_x S(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)d\tau\right\}\rho(\theta)$$

Finally, we make $\mu = t$ and so we obtain the solution of the original problem (2.74):

$$b_0(t,x,\eta,\theta) = \exp\left\{-\frac{1}{2m}\int_0^t \Delta_x S(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)d\tau\right\}\rho(\theta)$$

□

Theorem 2.22. *Let b_0 be defined as in (2.75) with $\rho(\theta) := e^{-|\theta|^2}\xi(\theta)$ and $\xi\in C_b^\infty(\mathbb{R}^k;\mathbb{R}^+)$. Then $b_0(t,x,\eta,\theta)\in C^\infty([0,T]\times\mathbb{R}^{2n+k};\mathbb{R}^+)$ and $b_0(t,x,\eta,\cdot)\in\mathcal{S}(\mathbb{R}^k;\mathbb{R}^+)$ for every (t,x,η) fixed. Moreover, there exists a constant $C^+(T)>0$ such that*

$$|\partial_x^\alpha b_0(t,x,\eta,\theta)| \ \leq\ C_\alpha^+(T)e^{d_\alpha(T)\lambda(x,\eta)}e^{-|\theta|^2} \quad \forall(x,\eta,\theta)\in\mathbb{R}^{2n+k} \tag{2.77}$$

Proof. Let us first obtain a more explicit expression for $(\Delta_x)S(\cdot)$:

$$\begin{aligned}
\Delta_x S(t,x,\eta,\theta) &= 2tr(L)t\ + \langle\Delta_x\nu(t,x,\theta),\theta\rangle + \langle v(t,x,\eta),\Delta_x f(t,x,\theta)\rangle\\
&+\ 2\langle\nabla_x v(t,x,\eta),\nabla_x f(t,x,\theta)\rangle + \Delta_x g(t,x,\theta)\\
&= 2tr(L)t\ + \langle 2R(t)\Delta_x f(t,x,\theta),\theta\rangle + \langle v(t,x,\eta),\Delta_x f(t,x,\theta)\rangle\\
&+\ 2\langle\nabla_x v(t,x,\eta),\nabla_x f(t,x,\theta)\rangle + \Delta_x g(t,x,\theta)\\
&= 2tr(L)t\ + \langle 2R(t)\Delta_x f(t,x,\theta),\theta\rangle + \langle v(t,x,\eta),\Delta_x f(t,x,\theta)\rangle\\
&+\ 2\langle\nabla_x v(t,x,\eta),\nabla_x f(t,x,\theta)\rangle + \Delta_x g(t,x,\theta)
\end{aligned} \tag{2.78}$$

Now, we recall that

$$\gamma^x(t,x,\theta)(\tau) = x - \int_\tau^t \theta^x(r) + f^x(t,x,\theta^x)(r)\ dr$$

where f and all its derivatives are L^2 uniformly bounded, as proved in Lemma 2.12, whereas v is linear in (x,η) and g is L^∞ bounded. Now we observe that by setting $\rho(\theta) := e^{-|\theta|^2}\xi(\theta)$ with a bounded $\xi \in C^\infty(\mathbb{R}^k;\mathbb{R}^+)$ then $b_0(t,x,\eta,\cdot)$ is a Schwartz function on $\mathbb{R}^k$. Indeed,

$$|b_0(t,x,\eta,\theta)| \leq \exp\left\{\frac{1}{2m}\int_0^t |\Delta_x S(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)|d\tau\right\}e^{-|\theta|^2}\xi(\theta)$$

But by the above detailed computation we see that

$$\begin{aligned}
&|\Delta_x S(\tau,\gamma^x(t,x,\theta),\eta,\theta)| \\
\leq\ & |2\mathrm{tr}(L)t| + 2\|R(t)\|\ \|\Delta_x f(t,\gamma^x,\theta)\|_{L^2}\|\theta\| + \|v(t,\gamma^x,\eta)\|_{L^2}\|\Delta_x f(t,\gamma^x,\theta)\|_{L^2} \\
+\ & 2\|\nabla_x v(t,\gamma^x,\eta)\|_{L^2}\|\nabla_x f(t,\gamma^x,\theta)\|_{L^2} + \|\Delta_x g(t,\gamma^x,\theta)\|_{L^\infty}
\end{aligned}$$

$\|\Delta_x f(t,\gamma^x(t,x,\theta),\theta)\|_{L^2}\|\theta\|$ is linear in θ and $\|v(t,\gamma^x(t,x,\theta),\eta)\|_{L^2}\|\Delta_x f(t,\gamma^x(t,x,\theta),\theta)\|_{L^2}$ has a linear uniform growth on (x,η,θ). To see this, remark that

$$\|v(t,\gamma^x(t,x,\theta),\eta)\|_{L^2} \leq \|v(t,x,\eta)\|_{L^2} + \|v(t,\int_\tau^t \theta^x(r)dr,\eta)\|_{L^2} + \|v(t,\int_\tau^t f^x(t,x,\theta^x)(r)dr,\eta)\|_{L^2}$$

The first and third term on the right hand side generate a linear growth on (x,η), the second term has a linear dependence on θ. The other terms above are bounded with respect to all variables. We conclude that b_0 has a uniform exponential behaviour on all its variables, and that the function $\rho(\theta) := e^{-|\theta|^2}\|\xi\|_{C^0}$ makes the effective dependence on θ of Schwartz type. □

Theorem 2.23. *Let S and Σ_S be as in Theorem 2.15. Then there exists $\widetilde{\Theta}_N \in C_b^\infty([0,T]\times\mathbb{R}^{2n+k};\mathbb{R})$ with $\widetilde{\Theta}_N|_{\Sigma_S} = 0$, such that the solution S_N of the problem*

$$\begin{cases} \partial_t b_{0,N} + \dfrac{1}{m}\nabla_x S_N\ \nabla_x b_{0,N} + \dfrac{1}{2m}\Delta_x S_N\ b_{0,N}(t,x,\eta,\theta) = \widetilde{\Theta}_N, \\ b_{0,N}(0,x,\eta,\theta) = \rho(\theta). \end{cases} \tag{2.79}$$

enjoys the property:

$$\Pi^j(\widetilde{\Theta}_N) \in C_b^\infty([0,T]\times\mathbb{R}^{2n+k};\mathbb{R}) \qquad \forall 1\leq j\leq N, \quad N=1,2,\ldots \tag{2.80}$$

where, as in Theorem 2.16:

$$\Pi(\widetilde{\Theta}_N) := \mathrm{div}_\theta\left(\widetilde{\Theta}_N\frac{\nabla_\theta S_N}{|\nabla_\theta S_N|^2}\right)$$

Proof. Let us define

$$b_{0,N}(t,x,\eta,\theta) := \exp\left\{-\frac{1}{2m}\int_0^t \Delta_x S_N(\tau,\gamma^x(t,x,\theta)(\tau),\eta,\theta)d\tau\right\}\rho(\theta) \tag{2.81}$$

and prove that is solves the above problem. Indeed, we can write down the expantions for $z := (x, \eta, \theta)$ around $\bar{z} \in \Sigma_{S_N} = \Sigma_S$

$$
\begin{aligned}
b_{0,N}(t,z) &= b_0(t,\bar{z}) + f_N(t,z) &(2.82)\\
\nabla_x b_{0,N}(t,z) &= \nabla_x b_0(t,\bar{z}) + g_N(t,z) &(2.83)\\
\partial_t b_{0,N}(t,z) &= \partial_t b_0(t,\bar{z}) + h_N(t,z) &(2.84)
\end{aligned}
$$

all these terms are related to the choice of G_N in Theorem 2.16 and their rate of convergence to zero near $\bar{z}$ are related as well. By unperturbed equation (2.74), we compute:

$$
\begin{aligned}
\widetilde{\Theta}_N(t,z) &= \partial_t b_{0,N} + \frac{1}{m}\nabla_x S_N \ \nabla_x b_{0,N} + \frac{1}{2m}\Delta_x S_N \ b_{0,N}(t,z)\\
&= \partial_t b_0(t,\bar{z}) + h_N(t,z) + \frac{1}{m}\left(\nabla_x S(t,\bar{z}) + F_N^x(t,z)\right)\left(\nabla_x b_0(t,\bar{z}) + g_N(t,z)\right)\\
&+ \frac{1}{2m}(\Delta_x S(t,\bar{z}) + G_N(t,z))(b_0(t,\bar{z}) + f_N(t,z))\\
&= h_N(t,z) + \frac{1}{m}\nabla_x S(t,\bar{z}) g_N(t,z) + F_N^x(t,z)\left(\nabla_x b_0(t,\bar{z}) + g_N(t,z)\right)\\
&+ \frac{1}{2m}\Delta_x S(t,\bar{z}) f_N(t,z) + \frac{1}{2m} G_N(t,z)(b_0(t,\bar{z}) + f_N(t,z)) \qquad (2.85)
\end{aligned}
$$

Moreover, by Theorem 2.16, we remember that around $\bar{z} \in \Sigma_{S_N} = \Sigma_S$ the new stationarity equation is

$$\nabla_\theta S_N(t,z) = F_N^\theta(t,z)$$

Now we can state that a suitable choice of F_N^θ, F_N^x and G_N leads to the following property:

$$\Pi^j(\widetilde{\Theta}_N) \in C_b^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R}) \qquad \forall 1 \le j \le N$$

□

3 A class of global FIO

In this section we follow the general setting of Hörmander [Ho], and in particular we study a class of FIO related to the Hamiltonian flow $\phi_{\mathcal{H}}^t$, by using the generating functions constructed in the previous section. The study of the topology of their critical points will be useful to determine important analitical properties of the FIO such as asymptotic behaviour of the kernel and L^2-continuity.

3.1 Basic definition and main properties

First, we introduce the set of phase functions:

Definition 3.1. *The set of phase functions* $S(t,x,\eta,\theta):[0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k\to\mathbb{R}$ *is the set of smooth global generating functions of the graphs* $\Lambda_t\subset T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n$ *of the canonical maps* $\phi^t_H:T^\star\mathbb{R}^n\to T^\star\mathbb{R}^n$*, with the inititial condition* $S(0,x,\eta,\theta)=\langle x,\eta\rangle$*. Each* Λ_t *admits the parametrization:*

$$\begin{aligned}\Lambda_t &:= \big\{(y,\eta;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n \mid (x,p)=\phi^t_{\mathcal{H}}(y,\eta)\big\}\\ &= \{(y,\eta;x,p)\in T^\star\mathbb{R}^n\times T^\star\mathbb{R}^n \mid p=\nabla_x S,\quad y=\nabla_\eta S,\quad 0=\nabla_\theta S(t,x,\eta,\theta)\}\end{aligned}$$

Before going further, we recall that by Theorem 2.17, the generating function S enjoys an important property. Namely, consider the set of critical points

$$\Sigma_S := \{(x,\eta,\theta)\in\mathbb{R}^{2n+k} \mid 0=\nabla_\theta S(t,x,\eta,\theta)\}. \tag{3.1}$$

Then Σ_S is a manifold globally diffeomorphic to Λ_t; moreover for all $t>0$ the following set

$$\Upsilon_S := \{(x,\eta,\theta)\in\mathbb{R}^{2n+k} \mid |x|^2+|\eta|^2>D(T)^2,\ |\theta|\le\tilde{K}_2(T)\lambda(x,\eta)\} \tag{3.2}$$

is free from critical points, i.e.:

$$\Upsilon_S\subset\mathbb{R}^{2n+k}\backslash\Sigma_S$$

Second, we introduce the relevant class of symbols associated to S:

Definition 3.2. *The set of symbols consists of all* $b\in C^\infty([0,T]\times\mathbb{R}^{2n}\times\mathbb{R}^k;\mathbb{R})$ *such that*

(i)

$$b(0,x,\eta,\theta)=\rho(\theta),\quad \rho(\cdot)\in\mathcal{S}(\mathbb{R}^k;\mathbb{R}^+),\quad \int_{\mathbb{R}^k}\rho(\theta)d\theta=1.$$

(ii) For all multi-indices α,β,σ *and* $t\in]0,T]$ *the inequalities*

$$|b(t,x,\eta,\theta)|\le\begin{cases} C^+(T)\ e^{\lambda(x,\eta)}e^{-|\theta|^2}, & (x,\eta,\theta)\notin\Upsilon_S\\[2ex] C^-(T)\lambda^{-n}(x,\eta)e^{-|\theta|^2}, & (x,\eta,\theta)\in\Upsilon_S\end{cases} \tag{3.3}$$

hold for some constants $C^{\pm}_{\alpha,\beta,\sigma}(T)>0$.

Remark 3.3. The exponential upper bound outside Υ_S is verified by the symbol b_0 (see Th. 2.22) and also, as we will see, by any other symbol $b_j, j=1,\dots$ entering in Theorem 1.1. Moreover, on domain Υ_S there are no critical points for the function S and this leads to require asymptotic vanishing behaviour of type $\lambda^{-n}(x,\eta)e^{-|\theta|^2}$ in this region for b_0; as a conseguence the same asymptotic property is fulfilled by all b_j. This setting is motivated by the fact that the contribution of this region to the FIO can be of order $O(\hbar^\infty)$ as we see in Corollary 3.7. In this framework, we provide a very simple proof of global L^2 continuity.

Finally, we introduce the class of global FIO associated to the Hamiltonian flow $\phi^t_{\mathcal{H}}$:

Definition 3.4. *Fix a phase function S as in Definition 3.1, and a symbol b as in Definition 3.2. Then the global $\hbar$-Fourier Integral Operator on $\mathcal{S}(\mathbb{R}^n)$ is defined as:*

$$B(t)\varphi(x) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}\ b(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy \tag{3.4}$$

In equivalent way, it can be rewritten in the form:

$$B(t)\varphi(x) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}\widetilde{S}(t,x,y,u)}\ \widetilde{b}(x,u)\ du\ \varphi(y)\ dy \tag{3.5}$$

where $u := (\eta,\theta)$, $\widetilde{S}(t,x,y,u) := S(t,x,\eta,\theta) - \langle y,\eta\rangle$ and $\widetilde{b}(t,x,u) := b(t,x,\eta,\theta)$. Indeed, if S generates the Lagrangian submanifold Λ, then $\widetilde{S}$ does the same in new variables:

$$\Lambda = \{(x,p;y,\eta) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x\widetilde{S},\quad \eta = -\nabla_y\widetilde{S},\quad 0 = \nabla_u\widetilde{S}\}$$

Theorem 3.5. *Let us consider the FIO as in Definition 3.4.*

$$B(t)\varphi(x) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}\ b(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy$$

Then $B(t) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$ is continuous and admits a continuous extension as an operator in $L^2(\mathbb{R}^n)$.

Proof. We begin by rewriting the FIO under the form of an integral operator acting on the $\hbar$-Fourier transform of the initial datum:

$$\begin{aligned} B(t)\varphi(x) &= (2\pi\hbar)^{-n} \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}\ b(t,x,\eta,\theta)\ d\theta\hat{\varphi}_\hbar(\eta)d\eta \\ &= (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} \widehat{\sigma}_\hbar(t,x,\eta)\hat{\varphi}_\hbar(\eta)d\eta. \qquad (3.6)\\ \widehat{\sigma}_\hbar(t,x,\eta) &:= \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}\ b(t,x,\eta,\theta)\ d\theta \end{aligned}$$

This is because of the integral in the θ-variables is absolutely convergent since $b(t,x,\eta,\cdot) \in \mathcal{S}(\mathbb{R}^k)$, and $\varphi(y)$ is also a Schwartz function and therefore admits a $\hbar$-Fourier transform in $\mathcal{S}(\mathbb{R}^n)$. The absolute convergence of the integral, as well as the L^2-continuity, is the consequence of the following computations.

$$\widehat{\sigma}_\hbar(t,x,\eta) = \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}\ b(t,x,\eta,\theta)\ d\theta = e^{\frac{i}{\hbar}\langle x,\eta\rangle}[\widehat{\sigma}^+_\hbar(t,x,\eta) + \widehat{\sigma}^-_\hbar(t,x,\eta)] \tag{3.7}$$

$$\widehat{\sigma}^-_\hbar(t,x,\eta) = \int_{B_\delta(0)\subset\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle x,\eta\rangle)}\ b(t,x,\eta,\theta)\ d\theta \tag{3.8}$$

$$\widehat{\sigma}^+_\hbar(t,x,\eta) = \int_{\mathbb{R}^k\backslash B_\delta(0)} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle x,\eta\rangle)}\ b(t,x,\eta,\theta)\ d\theta \tag{3.9}$$

with $\delta := \tilde{K}_2(T)\lambda(x,\eta)$. For $t=0$ we have $\widehat{\sigma}_\hbar^+(0,x,\eta)+\widehat{\sigma}_\hbar^-(0,x,\eta)=1$, $B(0)\varphi=\varphi$, and the continuity is obvious. For $t>0$ we can apply the estimates of Property (ii) of Definition 3.2. In the region containing the critical points we have:

$$\begin{aligned}|\widehat{\sigma}_\hbar^+(t,x,\eta)| &\leq \int_{\mathbb{R}^k\setminus B_\delta(0)} |b(t,x,\eta,\theta)|\ d\theta \leq \int_{\mathbb{R}^k\setminus B_\delta(0)} C_0^+(T)e^{\lambda(x,\eta)}e^{-|\theta|^2}d\theta \\ &= C_0^+(T)e^{\lambda(x,\eta)}\int_{\mathbb{R}^k\setminus B_\delta(0)} e^{-|\theta|^2}d\theta \end{aligned} \tag{3.10}$$

By writing down the integral in spherical coordinates, we have the following simple estimates

$$\int_{\mathbb{R}^k\setminus B_\delta(0)} e^{-|\theta|^2}d\theta = c_k\int_\delta^\infty e^{-\rho^2}\rho^{k-1}d\rho \leq c_k d_k(L)\int_\delta^\infty e^{-\rho L}d\rho = c_k d_k(L)e^{-L\delta}$$

for all $L>0$ and $d_k(L) := \sup_{\rho\geq 0} e^{-\rho^2}\rho^{k-1}e^{\rho L}$. In particular we choose $L := 1+\tilde{K}_2^{-1}(T)$, so that it follows

$$|\widehat{\sigma}_\hbar^+(t,x,\eta)| \leq C_0^+(T)e^{\lambda(x,\eta)}c_k d_k(L)e^{-\tilde{K}_2(T)\lambda(x,\eta)-\lambda(x,\eta)} = C_0^+(T)c_k d_k(L)e^{-\tilde{K}_2(T)\lambda(x,\eta)} \tag{3.11}$$

Whereas in the other region we can write:

$$\begin{aligned}|\widehat{\sigma}_\hbar^-(t,x,\eta)| &\leq \int_{B_\delta(0)\subset\mathbb{R}^k} |b(t,x,\eta,\theta)|d\theta \leq \int_{B_\delta(0)\subset\mathbb{R}^k} C_0^-(T)\lambda^{-n}(x,\eta)e^{-|\theta|^2}d\theta \\ &\leq \int_{\mathbb{R}^k} C_0^-(T)\lambda^{-n}(x,\eta)e^{-|\theta|^2}d\theta = C_0^-(T)\pi^{-\frac{k}{2}}\lambda^{-n}(x,\eta)\end{aligned} \tag{3.12}$$

We can now apply the Schur Lemma to both integral operators and this yields the L^2-boundedness. □

Now we prove a result, based on an argument of Duistermaat (see [Dui], Prop 2.1.1).

Lemma 3.6. *Let us consider a FIO of type (3.4) with phase function S and symbol g leading to a convergent integral. Suppose that*

$$\Pi(g) := \mathrm{div}_\theta\left(g\frac{\nabla_\theta S}{\|\nabla_\theta S\|^2}\right) \in C^\infty([0,T]\times\mathbb{R}^{2n}\times\mathbb{R}^k;\mathbb{R}) \tag{3.13}$$

and that the FIO with symbol $\Pi(g)$ is convergent. Then, the following equivalence holds:

$$\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}g(t,x,\eta,\theta)\ d\theta\hat{\varphi}(\eta)d\eta = -i\hbar\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}\Pi g(t,x,\eta,\theta)\ d\theta\hat{\varphi}(\eta)d\eta \tag{3.14}$$

Proof. The differential operator $\mathbb{L}\psi := \dfrac{\langle\nabla_\theta S,\nabla_\theta\psi\rangle}{\|\nabla_\theta S\|^2}$ verifies the relation

$$-i\hbar\mathbb{L}e^{\frac{i}{\hbar}S} = e^{\frac{i}{\hbar}S}$$

Now, by using integration by parts and the definition of the operator $\mathbb{L}$, we get:

$$\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S} g d\theta = -i\hbar \int_{\mathbb{R}^k} \mathbb{L}\left(e^{\frac{i}{\hbar}S}\right) g d\theta = -i\hbar \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S} \Pi(g) d\theta$$

□

Corollary 3.7. *Let* $\tilde{g} \in C^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R})$ *be such that* $\Pi^j(\tilde{g}) \in C^\infty([0,T] \times \mathbb{R}^{2n+k}; \mathbb{R})$ *and that the corresponding FIO is convergent for all* $0 \leq j \leq N$. *Then:*

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)} \tilde{g}(t,x,\eta,\theta)\ d\theta \hat{\varphi}(\eta) d\eta = (-i\hbar)^N \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)} \Pi^N \tilde{g}(t,x,\eta,\theta)\ d\theta \hat{\varphi}(\eta) d\eta$$

Proof. The iterated application of the previous Lemma gives the result. □

Remark 3.8. *If we take two symbols* g_1, g_2 *coinciding on* Σ_S *and moreover such that* $g_1 - g_2 = \tilde{g}$, $\tilde{g}$ *as in the above Corollary, then the related FIO coincide up to order* $O(\hbar^N)$.

4 Global parametrices of the evolution operator

Here we prove the main result of this paper. Consider the initial-value problem for Schrödinger equation

$$\begin{cases} i\hbar\partial_t \psi(t,x) = -\dfrac{\hbar^2}{2m}\Delta\psi(t,x) + V(x)\psi(t,x), \\ \\ \psi(0,x) = \varphi(x) \in \mathcal{S}(\mathbb{R}^n). \end{cases} \tag{4.1}$$

with a potential V quadratic at infinity, of the type (2.6).

We proceed to apply the results of the previous two sections in order to prove Theorem 1.1; namely, to construct a parametrix for the evolution operator under the form of series of a global FIO such that the solution of the Schrödinger equation (4.1) admits the following representation:

$$\psi(t,x) = \sum_{j=0}^{\infty} (2\pi\hbar)^{-n} \int_{\mathbb{R}^{2n+k}} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta) - \langle y,\eta\rangle)} \hbar^j b_j(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy + O(\hbar^\infty)$$

within the time interval $t \in [0,T]$ with T arbitrary large.

Proof of Theorem 1.1

Denoting $H_x := -\frac{\hbar^2}{2m}\Delta_x + V(x)$ the action of the Schrödinger operator we look for a family of global FIO $\{B_j(t)\}_{j \in \mathbb{N}}$ with symbol $b_j(t,x,\eta,\theta)$ enjoying Properties (i) and (ii) of Definition 3.4 such that

$$0 = (H_x - i\hbar\partial_t) \sum_{j=0}^{\infty} \int_{\mathbb{R}^{2n+k}} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta) - \langle y,\eta\rangle)} \hbar^j b_j(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy + O(\hbar^\infty)$$

First of all, the approximation of order zero is the operator $B_0(t)$ defined as:

$$B_0(t)\varphi := (2\pi\hbar)^{-n}\int_{\mathbb{R}^{2n+k}} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)} b_0(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy \tag{4.2}$$

It has to reduce to the identity for $t=0$ and to represent the semiclassical approximation of the propagator. To this end, the related phase function solves the H-J problem (2.53) and moreover the symbol b_0 solves the regularized geometric version of the transport equation as in Theorem 2.23. As we observed in Remark 3.3, we require that in the region Υ_S free from critical points of S, the symbol b_0 behaves as $\lambda^{-n}(x,\eta)e^{-|\theta|^2}$.
Now, we easily see that

$$\begin{aligned}&(H_x - i\hbar\partial_t)\, e^{\frac{i}{\hbar}S}b_0\\ &= e^{\frac{i}{\hbar}S}\left[\hbar^0\left(\frac{|\nabla_x S|^2}{2m}+V(x)+\partial_t S\right)b_0 - i\hbar^1\left(\partial_t b_0+\nabla_x S\ \nabla_x b_0+\frac{\Delta_x S}{2m}b_0\right)-\frac{\hbar^2}{2m}\Delta_x b_0\right]\end{aligned}$$

The first two symbols of this sum vanish on the critical points set Σ_S in such a way we can apply Corollary 3.7, and so they realize bounded operators of order $O(\hbar^\infty)$. As a consequence,

$$(H_x - i\hbar\partial_t)\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}b_0 d\theta\hat{\varphi}_\hbar(\eta)d\eta = -\frac{\hbar^2}{2m}\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}\Delta_x b_0 d\theta\hat{\varphi}_\hbar(\eta)d\eta + O(\hbar^\infty). \tag{4.3}$$

The operator $B_1(t)$ and the related symbol b_1 fulfill the analogous relation:

$$\begin{aligned}&(H_x - i\hbar\partial_t)\, e^{\frac{i}{\hbar}S}\hbar b_1\\ &= e^{\frac{i}{\hbar}S}\left[\hbar\left(\frac{|\nabla_x S|^2}{2m}+V(x)+\partial_t S\right)b_1 - i\hbar^2\left(\partial_t b_1+\nabla_x S\ \nabla_x b_1+\frac{\Delta_x S}{2m}b_1\right)-\frac{\hbar^3}{2m}\Delta_x b_1\right]\end{aligned}$$

The transport equation we now require for this symbol is the following:

$$\begin{cases} \partial_t b_1 + \nabla_x S\ \nabla_x b_1 + \dfrac{1}{2m}\Delta_x S\ b_1 = \dfrac{i}{2m}\Delta_x b_0, \\ \\ b_1(0,x,\eta,\theta) = 0. \end{cases} \tag{4.4}$$

As a consequence,

$$(H_x - i\hbar\partial_t)\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}(b_0+\hbar b_1) d\theta\hat{\varphi}_\hbar(\eta)d\eta = -\frac{\hbar^3}{2m}\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}\Delta_x b_1 d\theta\hat{\varphi}_\hbar(\eta)d\eta + O(\hbar^\infty)$$

The equation for the second order symbol:

$$\begin{cases} \partial_t b_2 + \nabla_x S\ \nabla_x b_2 + \dfrac{1}{2m}\Delta_x S\ b_2 = \dfrac{i}{2m}\Delta_x b_1, \\ \\ b_2(0,x,\eta,\theta) = 0. \end{cases}$$

implies

$$(H_x - i\hbar\partial_t)\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}(b_0+\hbar b_1+\hbar^2 b_2) d\theta\hat{\varphi}_\hbar(\eta)d\eta = -\frac{\hbar^4}{2m}\int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}S}\Delta_x b_2 d\theta\hat{\varphi}_\hbar(\eta)d\eta + O(\hbar^\infty)$$

Therefore we can deal with functions b_j, $j \geq 1$ fulfilling the recurrent equations

$$\begin{cases} \partial_t b_j + \nabla_x S \ \nabla_x b_j + \dfrac{1}{2m}\Delta_x S \ b_j = \dfrac{i}{2m}\Delta_x b_{j-1}, \\ \\ b_j(0,x,\eta,\theta) = 0. \end{cases} \tag{4.5}$$

Each solution b_j is a symbol as in Definition 3.2 and therefore (thanks to Th. 3.5) it defines a bounded operator $B_j(t)$. The same holds true for the remainder operators:

$$\mathcal{R}_j(t)\varphi = (2\pi\hbar)^{-n} \int_{\mathbb{R}^{2n+k}} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)} \hbar^{2+j} r_j(t,x,\eta,\theta) \ d\theta \ d\eta \ \varphi(y) \ dy$$

where $r_j := \dfrac{i}{2m}\Delta_x b_j$. In order to prove it, we need the following

Lemma 4.1. *For all $j \geq 1$ the solution of equation (4.5) fulfills the estimates:*

$$|b_j|, |\Delta_x b_j|(t,x,\eta,\theta) \leq \begin{cases} C_j^+(T) e^{d_j(T)\lambda(x,\eta)} e^{-|\theta|^2}, & (x,\eta,\theta) \notin \Upsilon_S \\ \\ C_j^-(T) \lambda^{-n}(x,\eta) e^{-|\theta|^2}, & (x,\eta,\theta) \in \Upsilon_S. \end{cases} \tag{4.6}$$

Proof. We consider the following problem

$$\begin{cases} \dfrac{d}{d\tau}\zeta(t,x,\eta,\theta)(\tau) = \nabla_x S(t, \zeta(t,x,\eta,\theta)(\tau), \eta, \theta) \\ \\ \zeta(t,x,\eta,\theta)(t) = x \end{cases} \tag{4.7}$$

and define

$$\Phi(\tau,x,\eta,\theta) := \exp\left\{ -\frac{1}{2m} \int_0^\tau \Delta_x S(t, \zeta(t,x,\eta,\theta)(r), \eta, \theta) dr \right\}$$

in order to apply the theory of characteristics ((θ,η) fixed) and find the solution:

$$b_j(t,x,\eta,\theta) = \frac{i}{2m} \int_0^t \Phi(t-\tau,x,\eta,\theta) \Delta_x b_{j-1}(\tau, \zeta(t,x,\eta,\theta)(\tau), \eta, \theta) d\tau \tag{4.8}$$

By the iteration of this map, we have a direct linear relationship between $\Delta_x b_0$ and b_j. Now we recall the estimates on b_0 proved in Theorem 2.22

$$|\partial_x^\alpha b_0(t,x,\eta,\theta)| \leq C_\alpha^+(T) e^{d_\alpha(T)\lambda(x,\eta)} e^{-|\theta|^2} \quad \forall (x,\eta,\theta) \in \mathbb{R}^{2n+k}$$

and the explicit analytic structure of S studied in Theorem 2.13:

$$\begin{aligned} S &= \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle Q(t)\theta,\theta\rangle + \langle v(t,x,\eta), \theta + f(t,x,\theta)\rangle + \langle \nu(t,x,\theta),\theta\rangle \\ &+ g(t,x,\theta) \end{aligned} \tag{4.9}$$

which implies the exponential behaviour of Φ. The exponential upper bound for $|b_j|$ and $|\Delta_x b_j|$ follows directly from that. In the region Υ_S we recall the upper bound of type $\lambda^{-n}(x,\eta)e^{-|\theta|^2}$

we required for $\Delta_x b_0$ and the expansion $\Delta_x S(z) = \Delta_x S(\bar{z}) + G(z)$ with $G \in C_b^\infty$ (see Th. 2.16). By using (4.8) we obtain this second estimate also for $|b_j|$ and $|\Delta_x b_j|$. □

As a consequence, we can apply the boundedness result of Theorem 3.5 and state the existence of constants $K_j(T) > 0$ such that $\|\mathcal{R}_j(t)\| \leq K_j(T)\hbar^{2+j}$. By well known arguments related to the Duhamel formula we obtain the estimate:

$$\left\| U(t) - \sum_{j=0}^{N} B_j(t) \right\| \leq \frac{1}{\hbar} \int_0^t \|\mathcal{R}_N(s)\| \, ds \leq T K_N(T) \hbar^{N+1}, \quad t \in [0,T].$$

□

Now we clarify the relationship between the construction of the previous theorem and Chazarain's formulation [Ch], as well as with the integral representation of Fujiwara [Fu].

Theorem 4.2. *Let $t \in [0,t_0]$, with t_0 so small that the solution of the Hamilton-Jacobi equation does not develop caustics. Consider the construction of Theorem 1.1, truncated at any finite order J:*

$$\sum_{j=0}^{J} B_j(t)\varphi := \sum_{j=0}^{J} (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta) - \langle y,\eta \rangle)} \hbar^j b_j(t,x,\eta,\theta) \, d\theta \, d\eta \, \varphi(y) \, dy \quad (4.10)$$

Then:

1. $$\sum_{j=0}^{J} B_j(t)\varphi = \sum_{\alpha=0}^{J} U_\alpha^{ch}(t)\varphi + O(\hbar^{J+1}) \quad (4.11)$$

   Here $U_\alpha^{ch}(t)$ is the term of order $\hbar^\alpha$ of Chazarain's FIO ([Ch]).

2. $$\sum_{j=0}^{J} B_j(t)\varphi = \sum_{\alpha=0}^{J} U_\alpha^{F}(t)\varphi + O(\hbar^{J+1}) \quad (4.12)$$

   where this time $U_\alpha^F(t)$ is the term of order $\hbar^\alpha$ of Fujiwara's integral operator ([Fu]).

Proof. In order to prove the first assertion, the main idea is to apply the stationary phase theorem to the oscillatory integrals (4.10) with respect to θ-variables. In the same way, if we consider the stationarity argument with respect to (θ,η)-variables we obtain the second assertion.

In the small time regime $t \in [0,t_0]$ there exists a unique smooth and global critical point $\theta^\star(t,x,\eta)$, solution of $0 = \nabla_\theta S(t,x,\eta,\theta)$. This fact suggests us to consider the translated phase function around this point $S(t,x,\eta,\theta + \theta^\star(t,x,\eta))$ with $\theta \in B_1(0)$ and symbol b_0 (see

Theorem 1.1) for which we choose the regularizing part as $\rho(\theta) := (volB_1(0))^{-1}\mathcal{X}_1(\theta)$, a C^∞ cut off function for the ball $B_1(0)$. The compact behaviour of b_j on the θ-variables follows as a consequence. The uniqueness of $\theta^\star$ and the compact setting in the oscillatory integral allow us to apply the stationary phase theorem to each integral in the θ-variables

$$B_j(t,x,\eta) = \int_{\mathbb{R}^k} e^{\frac{i}{\hbar}S(t,x,\eta,\theta)}\hbar^j b_j(t,x,\eta,\theta)\ d\theta$$

obtaining

$$B_j(t,x,\eta) = e^{\frac{i}{\hbar}S(t,x,\eta,\theta^\star)}|\det\nabla^2_\theta S(t,x,\eta,\theta^\star(t,x,\eta))|^{-\frac{1}{2}}\ e^{\frac{i\pi}{4}\sigma}\hbar^j b_j(t,x,\eta,\theta^\star) + O(\hbar^{j+1}) \quad (4.13)$$

where $\sigma = sgn\nabla^2_\theta S(t,x,\eta,\theta^\star(t,x,\eta))$ and we have omitted (to simplify the exposition) the explicit form of the higher orders symbols. Now we remark that the function $S(t,x,\eta,\theta^\star)$ equals the phase used in the Chazarain's paper (the action functional evaluated on the classical curve with boundary conditions x and η). Hence, by the uniqueness of the symbol expansion of the propagator in powers of $\hbar$, we get the corrispondence between the symbols obtained as in (4.13) and the ones obtained in the above-mentioned paper. This implies the equivalence of the two series (4.11) up to an order $o(\hbar^{J+1})$. By the same argument, applied this time to the integrals over $u := (\theta,\eta)$ and $\Phi(t,x,y,u) := S(t,x,\eta,\theta) - \langle y,\eta\rangle$

$$\widetilde{B}_j(t,x,y) = \int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}\hbar^j b_j(t,x,\eta,\theta)\ d\theta\ d\eta = \int_{\mathbb{R}^{n+k}} e^{\frac{i}{\hbar}\Phi(t,x,y,u)}\hbar^j\widetilde{b}_j(t,x,u)du$$

we use the uniqueness of the critical point $u^\star(t,x,y)$. to get

$$\widetilde{B}_j(t,x,y) = e^{\frac{i}{\hbar}\Phi(t,x,y,u^\star)}\hbar^j|\det\nabla^2_\theta\Phi(t,x,y,u^\star(t,x,y))|^{-\frac{1}{2}}e^{\frac{i\pi}{4}\sigma}\ \widetilde{b}_j(t,x,u^\star(t,x,y)) + O(\hbar^{j+1})$$

The phase function $\Phi(t,x,y,u^\star)$ is the same used by Fujiwara and therefore also (4.12) is proved. This concludes the proof of the Theorem. □

5 Multivalued WKB semiclassical approximation

In this final section we prove Theorem 1.2, mainly applying the Stationary Phase theorem to the global FIO (4.2), in order to get a multivalued WKB semiclassical approximation of the Schrödinger evolution operator.

Proof of Theorem 1.2

We start by recalling that (as proved in Theorem 1.1) the $\hbar$-Fourier Integral Operator

$$B_0(t)\varphi := (2\pi\hbar)^{-n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{\frac{i}{\hbar}(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}b_0(t,x,\eta,\theta)\ d\theta\ d\eta\ \varphi(y)\ dy \quad (5.1)$$

is a semiclassical approximation of the Schrödinger propagator for all $t \in [0, T]$. Under the particular hypothesis

$$V(x) = \frac{1}{2}|x|^2 + V_0(x), \quad \sup_{x \in \mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1, \quad t \neq (2\tau + 1)\frac{\pi}{2} \ (\tau \in \mathbb{N}),$$

we proved (see Theorems 2.18, 2.19 and 2.20) that the phase function has isolated and finitely many critical points; precisely the equation

$$\nabla_\theta S(t, x, \eta, \theta) = 0 \tag{5.2}$$

is solved on a finite open partition $(x, \eta) \in \mathbb{R}^{2n} = \bigcup_{\ell=1}^{\mathcal{N}(t)} D_\ell$ in such a way that on each D_ℓ there are exactly ℓ smooth solutions $\theta^\star(t, x, \eta)$, $1 \leq \alpha \leq \ell$. This property allows us to apply the Stationary Phase Theorem (see [Ho2] vol. I) to the oscillatory integral in (5.1). The result is:

$$\begin{aligned} B_0(t, x, \eta)\Big|_{D_\ell} &= \int_{\mathbb{R}^k} e^{\frac{i}{\hbar} S(t,x,\eta,\theta)} b_0(t, x, \eta, \theta)\, d\theta \\ &= \sum_{\alpha=1}^{\ell} e^{\frac{i}{\hbar} S(t,x,\eta,\theta^\star_\alpha(t,x,\eta))} |\det \nabla^2_\theta S(t, x, \eta, \theta^\star_\alpha(t, x, \eta))|^{-\frac{1}{2}} e^{\frac{i\pi}{4}\sigma_\alpha} b_0(t, x, \eta, \theta^\star_\alpha(t, x, \eta)) \\ &+ O(\hbar) \end{aligned}$$

where $\sigma_\alpha = sgn \nabla^2_\theta S(t, x, \eta, \theta^\star_\alpha(t, x, \eta))$. In the small time regime $t \in [0, t_0]$ and for potentials V quadratic at infinity, it is well known (see i.e. [We]) that the graph of the Hamiltonian flow

$$\begin{aligned} \Lambda_t &:= \big\{(y, \eta; x, p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid (x, p) = \phi^t_{\mathcal{H}}(y, \eta)\big\} \\ &= \{(y, \eta; x, p) \in T^\star\mathbb{R}^n \times T^\star\mathbb{R}^n \mid p = \nabla_x S, \ y = \nabla_\eta S, \ 0 = \nabla_\theta S\} \end{aligned}$$

is globally transverse to the base manifold $(x, \eta) \in \mathbb{R}^{2n}$, so the equation (5.2) admits a unique global smooth solution $\theta^\star(t, x, \eta)$. This simplified setting yields:

$$\begin{aligned} B_0(t, x, \eta) &= e^{\frac{i}{\hbar} S(t,x,\eta,\theta^\star(t,x,\eta))} \ |\det \nabla^2_\theta S(t, x, \eta, \theta^\star(t, x, \eta))|^{-\frac{1}{2}} \ e^{\frac{i\pi}{4}\sigma} \ b_0(t, x, \eta, \theta^\star(t, x, \eta)) \\ &+ O(\hbar) \end{aligned}$$

which is the usual WKB construction, local in time. □

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