The Semi-classical Trace Formula and Propagation of Wave Packets

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Contents

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Abstract

We study spectral and propagation properties of operators of the form $S_\hbar = \sum_{j=0}^N \hbar^j P_j$ where $\forall j$ P_j is a differential operator of order j on a manifold M, asymptotically as $\hbar \to 0$. The estimates are in terms of the flow $\{\phi_t\}$ of the classical Hamiltonian $H(x,p) = \sum_{j=0}^N \sigma_{P_j}(x,p)$ on T^*M, where σ_{P_j} is the principal symbol of P_j. We present two sets of results. (I) The "semiclassical trace formula", on the asymptotic behavior of eigenvalues and eigenfunctions of $S_\hbar$ in terms of periodic trajectories of H. (II) Associated to certain isotropic submanifolds $\Lambda \subset T^*M$ we define families of functions $\{\psi_\hbar\}$ and prove that $\forall t$ $\{\exp(-it\hbar S_\hbar)(\psi_\hbar)\}$ is a family of the same kind associated to $\phi_t(\Lambda)$.

Introduction and description of results.

In this paper we present some results concerning spectral and propagation properties of a class of differential operators "with small parameter", $\hbar$ (Planck's constant). We have in mind operators of the form $a(x, \hbar D_x)$ on a compact manifold (or on $\mathbb{R}^n$ under additional assumptions at infinity) where $a(x,p)$ is a polynomial in p bounded below. We are interested in trace formulae, localization of eigenfunctions and propagation of wave packets in the semi-classical limit, that is as $\hbar$ tends to zero. We present two sets of results: (A) The Theorems we announced in [32], including a rigorous proof of a version of the Gutzwiller trace formula, and (B) a general definition of "wave packets" on arbitrary manifolds and a theorem on their propagation under the time-dependent Schrödinger equation. A secondary goal of this paper is to show how semi-classical problems can be treated with *standard* Fourier integral operator methods. We first learned of this possibility while reading an article of Yves Colin de Verdière, [7], (proof of Theorem 4.4). A first version of the Gutzwiller trace formula was obtained by this method in joint work of one of us with Victor Guillemin, see [19], in the course of studying elliptic operators with symmetries. This approach, which we believe is very natural (e.g. its underlying geometry is that of the pre-quantum circle bundle) is developed here systematically.

The apparent reason that Hörmander's theory of Lagrangian distributions seems unsuited to the treatment of semi-classical problems is that it is a *homogeneous* theory. That is, in Hörmander's theory all geometrical objects (e.g. Lagrangian submanifolds, symbols) are homogeneous under the $\mathbb{R}^+$ action on the punctured cotangent bundle of the manifold where they live. This is clearly false of the corresponding semi-classical objects. Homogeneity is however restored if one assigns to $\hbar$ the order (-1). (Because each x derivative has a factor of $\hbar$.) The Schrödinger operator becomes then formally of order zero, and therefore the fundamental solution of Schrödinger's equation $i\hbar\partial u/\partial t = a(x, \hbar D_x)u$ is the exponential of an operator of formal order one, namely $-i\hbar^{-1}a(x, \hbar D_x)$. In our method we *in fact* realize $\hbar$ as a pseudodifferential operator of order (-1), microlocally in a region of bounded energy. This in particular leads to the proof of the trace formulae of [32].

To be more specific, consider a Schrödinger operator on, say, a compact manifold M, -$\hbar^2\Delta$ + V(x), where Δ denotes the Laplacian on M. The time dependent Schrödinger equation is

$$\hbar\, i\, \frac{\partial \psi_\hbar}{\partial t} = (-\hbar^2\Delta + V(x))\psi_\hbar\ . \tag{1}$$

One is interested in the initial value problem with initial condition $\psi_\hbar^0$ in $L^2(M)$. Since we are interested in asymptotics as $\hbar \to 0$, it is natural to prescribe the small $\hbar$ behavior of the initial data, $\psi_\hbar^0$. We shall do this by considering the $\hbar$ *transform* of the initial data, which by definition is the Fourier transform in $\hbar^{-1}$, that is, the following distribution on $M \times S^1$:

$$\Psi^0(x,\theta) = \sum_{m=1}^{\infty} \psi_{1/m}(x)\, e^{im\theta}\ . \tag{2}$$

In making this definition, we have tacitly restricted $\hbar$ to take the values $1/m$, for $m = 1, 2, \ldots.$ We'll see later on that in many cases this restriction on $\hbar$ can be lifted.

Definition 0.1 *We will say that the family $\{\psi_\hbar^0\}$ is of* semi-classical type *iff the wave-front set of (2) is contained in the set $\{\ \kappa \neq 0\ \}$, where κ is the variable dual to θ.*

Let us give two examples of such families:
A. Wave packets (§5): let us consider the function

$$\phi^\hbar_{(q,p,A)}(x) = (\det A_i)^{1/4} e^{-iq.p/2\hbar} e^{-(x-q)^t A(x-q)/\hbar} e^{ip.x/\hbar} \ .$$

Then the wave front set of

$$\Psi(\theta, x) = \sum_{m=1}^{\infty} \psi^{m^{-1}}_{(q,p,A)}(x) e^{im\theta}$$

is the set $\{(q, \theta = -qp/2; \kappa p, \kappa), \kappa > 0\}$.
B. WKB states. Consider now a family of vectors of the form $\psi_\hbar(x) = e^{iS(x)}$,with S(x) real on an open set, then the wave front set of $\Psi(\theta, x)$ defined as before is:

$$\{\ (\theta, x; \kappa, \xi)\ ;\ \xi = \kappa S'(x)\ ,\ \kappa > 0\ ,\ \theta = S(x)\ \}\ .$$

Back to the time-dependent Schrödinger equation, (1), if we denote by Ψ the $\hbar$-transform of the time-dependent wave functions $\psi_\hbar$, one easily sees that the equation is equivalent, formally, to

$$-D_t \Psi = D_\theta[-(D_\theta^{-1})^2 \Delta + V(x)]\Psi = [-D_\theta^{-1}\Delta + D_\theta V(x)]\Psi \tag{3}$$

where D_θ^{-1} is a parametrix of D_θ, which will be properly defined later. One of the main ideas of this paper consists in noting that the operator

$$P = -D_\theta^{-1}\Delta + D_\theta V(x) \tag{4}$$

can be considered *when acting on semi-classical families* as a classical pseudo-differential operator on $M \times S^1$ with symbol

$$p(x, \theta; \xi, \kappa) = \kappa^{-1}\xi^2 + \kappa V(x)\ . \tag{5}$$

In fact, notice that p is homogeneous of degree one in the cotangent variable (ξ, κ). Of course one has to deal with the fact that κ^{-1} is singular, and that besides that $\kappa^{-1}\xi^2$ looks not like a classical symbol, but like a product-type symbol. However, we will see that, micro locally inside cones of the form

$$\|\xi\|\kappa^{-1} < C$$

and away from $\kappa = 0$, P can be treated as a first order classical pseudo-differential operator. Somewhat more precisely, the operator P will behave on families of semi classical type as a first order operator, up to an error of size $O(\hbar^\infty)$. This heuristic discussion is valid for any differential operator of the form $a(x, \hbar D_x)$ and is made mathematically precise in §3. In §1 we analyze its geometrical meaning; as we will see that the classical version of the $\hbar$ transform is the pre-quantum circle bundle of the initial phase space (this section is however not needed in the proofs of the main results).

Let us mention that the idea of taking the Fourier (Laplace) transform in the variable $1/\hbar$ is also present in the study of Borel summability of semi-classical expansions, as developed by André Voros, see [39].

A summary of the results of the paper is the following:

- The semi-classical trace formula (Theorem 5.3 announced in [32] (see also works of Meinrenken [30] and Dozias [11] for the case M=$\mathbb{R}^n$)): this is the main result of the paper and was actually the first motivation of the formalism. In §6 we describe several variants: relationship with Bohr Sommerfeld conditions, uniformity of the estimates in the energy, and the case where the flow is completely periodic (for the latter see also Dozias, [12]).

- Global $\hbar$-Fourier Integral Operators (§3; see also [30] and [11]): we describe a theory of global Fourier integral operators with small parameter valid on manifolds. This includes the propagator of the Schrödinger operator, suitably microlocalized.
- Construction of Lagrangian semi-classical states and wave packets (and more general semi-classical states) on a Riemannian manifold (§2). We construct intrinsic Gaussian wave packets on manifolds and describe the action of Fourier integral operators on them. (For an independent theory, see Karasev's work, [27].)

Finally, in the appendix we observe that with our methods one can easily construct semiclassical pseudodifferential operators on manifolds. One immediately has an Egorov type theorem, and the uniformity of distribution of eigenfunctions in the ergodic case can be proved as in Colin de Verdière's work, [8], thereby obtaining as a corollary the manifold version of a result of Helffer, Martinez and Robert, ([23]).

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1 Preliminaries

1.1 Physical motivation.

Our objective in this subsection is to motivate our approach to semi-classical analysis by some general considerations in physical language. The basic idea of our approach is to take $1/\hbar$ as a dynamical variable and not just as a parameter. Although we can't motivate this a priori, we feel that the considerations below justify this approach a posteriori. In the end this is just a philosophical issue; the concrete results of the method are the estimates derived in subsequent sections.

Let M be the configuration space of a mechanical system, and $L : TM \to \mathbb{R}$ a Lagrangian. Here TM is the tangent bundle of M. In [10], Dirac argued that the quantum analogue of the classical Action, $S = \int_\gamma L dt$, is as follows:

$$\langle\, q'_{t+\delta t} \mid q_t \,\rangle \;\sim\; e^{i\kappa S} \,, \tag{6}$$

where here and in what follows

$$\boxed{\kappa \;=\; \tfrac{1}{\hbar}}$$

and in (6) S is regarded as a function of the endpoints, q' and q, of the classical trajectory γ which at time t passes through q and at time $t+\delta t$ passes through q'. This was to become later on the starting point of Feynman's derivation of the formula for the propagator as a path integral.

Of formula (6) we presently focus on the following principle: *To introduce Planck's constant $\hbar$ in mechanics, divide the Lagrangian L by $\hbar$.* This obviously does not change the classical equations of motion, since in the Euler-Lagrange equations for $\hbar^{-1}L$ we can cancel out the $\hbar$. However, keeping $\hbar$ in gives, on the Hamiltonian side, different-looking equations of motion. In this section we will keep track of $\hbar$ on the Hamiltonian side, and shortly will take κ itself as a dynamical variable. We will see that this is naturally related to the concept of pre-quantum bundle of Kostant and Souriau.

To illustrate what happens if L is multiplied by κ on the Hamiltonian side, we begin with a Lagrangian of the classical type, $L(q\,,\,\dot q)$, which we then proceed to multiply by $\kappa = 1/\hbar$. The associated momenta are now

$$\xi_i \;=\; \kappa\, p_i \,, \tag{7}$$

where

$$p_i \;=\; \frac{\partial L(q,\dot q)}{\partial \dot q_i} \tag{8}$$

are the original classical momenta. It follows from this and a simple calculation that the new Hamiltonian is

$$\mathcal{H}(q,\xi) \;=\; \xi \cdot \dot{q} - L(q,\dot{q}) = \;\kappa\, H(q,p), \tag{9}$$

where $H(q,p)$ is the Hamiltonian associated to the original Lagrangian, while the symplectic form $\omega_\kappa = \sum dq^i \wedge d\xi_i$ is equal to the symplectic form defined by the original Hamiltonian, $\sum dq^i \wedge dp_i$ multiplied by κ. Thus the change of variables (we will keep the notation throughout)

$$\boxed{\xi = \kappa p}$$

transforms the Hamilton vector field of $\mathcal{H}$, ω_κ into the Hamilton vector field of H, ω.

In our approach to semi-classical analysis, *we regard κ as a dynamical variable.* Introducing a new variable, θ, the variable conjugate to κ, consider (9) as a Hamiltonian of all the variables:

$$\mathcal{H} \;=\; \mathcal{H}(q,\xi;\theta,\kappa) \;=\; \kappa\, H(q,p) \quad \text{where} \quad p \;=\; \kappa^{-1}\xi. \tag{10}$$

This is a well-defined function on the manifold

$$\Sigma \;=\; T^*M \times \mathbb{R} \times \mathbb{R}^+ \tag{11}$$

which we endow with the symplectic form

$$\omega + d\theta \wedge d\kappa\ , \tag{12}$$

where $\omega = \sum dq \wedge d\xi$ is the *standard* symplectic form on T^*M (independent of $\hbar$!). Notice that Σ is a symplectic cone: $\mathbb{R}^+$ acts on it by the recipe

$$\forall r \in \mathbb{R}^+ \quad r \cdot (x,\xi;\theta,\kappa) \;=\; (x, r\xi;\theta, r\kappa) \tag{13}$$

and $r^*\omega \;=\; r\,\omega$. Also notice that $\mathcal{H}$ is homogeneous of degree one with respect to this action. *Thus we have homogenized the problem.*

Hamilton's equations for $\mathcal{H}$ in Σ are

$$\dot{q} \;=\; \frac{\partial H}{\partial p}(q,p)\ , \tag{14}$$

$$\dot{\xi} \;=\; -\kappa\,\frac{\partial H}{\partial q}(q,p), \tag{15}$$

$$\dot{\theta} \;=\; H(q,p) - p \cdot \frac{\partial H}{\partial p}(q,p)\ , \tag{16}$$

$$\dot{\kappa} \;=\; 0\ . \tag{17}$$

The first two equations are equivalent to Hamilton's equations for H, since $\xi = \kappa p$. *It follows that the third equation says that θ evolves according to minus the initial Lagrangian $-L$.*

The symplectic manifold Σ can also be seen to arise from the Lagrangian

$$\mathcal{L} \;=\; rL(q,\dot{q}) + \theta\dot{\kappa}\ , \tag{18}$$

which is a Lagrangian on the Cartesian product of M and a two dimensional space $\mathcal{C}$ with coordinates (θ,κ). This Lagrangian is singular in the sense that the Legendre transformation associated with it is not invertible. However, the image of the Legendre transformation is easily seen to be a symplectic submanifold of the cotangent bundle of $M \times \mathcal{C}$ naturally identifiable with Σ, and the Hamiltonian there is precisely $\mathcal{H}$. Moreover, the canonical one-form on Σ coming from the Lagrangian $\mathcal{L}$, namely

$$\alpha \;:=\; \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}^i}\, dq^i \;+\; \frac{\partial \mathcal{L}}{\partial \dot{\theta}}\, d\theta\ , \tag{19}$$

is equal to

$$\alpha \;=\; \kappa \sum_i \; p_i \; dq^i \;+\; \kappa d\theta \;, \tag{20}$$

that is, the canonical one-form on the cotangent bundle of $M \times \mathbb{R}$. The natural action of the multiplicative group, $\mathbb{R}^+$, on Σ is Hamiltonian with Hamiltonian κ. The subset of Σ,

$$P \;:=\; \{\kappa = 1\}$$

is a principal $\mathbb{R}^+$ bundle over T^*M and the pull-back of (20) to P is a connection form whose curvature is precisely $-\omega$. *Thus P, α is the pre-quantum bundle of T^*M, with structure group $\mathbb{R}^+$.* We will investigate more closely the relationship between Σ and the pre-quantum bundle in the next subsection.

The quantization of these classical considerations consists, as usual, to associate to Σ a Hilbert space of functions defined on $M \times \mathbb{R}$. Since Σ is an open set in $T^*(M \times \mathbb{R})$, it is natural to take the Hilbert space $L^2(M \times \mathbb{R})$, (although for technical reasons it is sometimes useful to replace $\mathbb{R}$ by a circle group). If we follow the usual rules for the quantization of operators, namely

$$q \to \times q \tag{21}$$

$$p \to -i\,\nabla_q \tag{22}$$

$$e^{i\theta} \to \times e^{i\theta} \tag{23}$$

$$\kappa \to -i\frac{\partial}{\partial\theta} \;, \tag{24}$$

then, formally, the quantization of $\mathcal{H}(q,p;\theta,\kappa)$ is (up to usual ordering problems)

$$\mathcal{H} = -i\frac{\partial}{\partial\theta} \circ h\left(q\,,\, (-i\frac{\partial}{\partial\theta})^{-1}(-i)\,\nabla_{\partial/\partial q}\right) \;. \tag{25}$$

The next section will be devoted to a precise definition of this operator and to its microlocal properties, assuming given a quantization of the original classical Hamiltonian $H(q,p)$.

The quantum states on which the quantization of $\mathcal{H}$ operates can be written, after Fourier transformation in θ, in the form

$$\Psi(q,\theta) = \int \psi_\kappa(q)\; e^{i\kappa\theta}\; d\kappa \;. \tag{26}$$

The quantization of $\mathcal{H}$ commutes with ∂_θ, and so it preserves this decomposition. In fact each component corresponding to a given value of κ is of the form $e^{i\kappa\theta}\,\psi_\kappa(q)$, where ψ_κ is the usual wave function with $\hbar = 1/\kappa$. Conversely, given a family of states ψ_κ depending on $\hbar$, we can form Ψ given by (26). We will call Ψ the *$\hbar$-transform* of the family. Thus the $\hbar$ transform is the quantum analogue of the geometrical homogenization procedure described above. We will make this analogy more precise in §2. We close this section with a remark on the physical meaning of the phase θ: If we remember that the evolution of the variable θ is given by the action along classical trajectories, we can interpret the phase factor $e^{i\kappa\theta}$ as the semi-classical phase of the wave function, as defined in the early days of quantum mechanics.

1.2 The semi-classical homogenization of (T^*M, ω)

In the previous section we were led to consider the conic symplectic manifold

$$\Sigma \;=\; T^*(M \times \mathbb{R})^+ \;:=\; \{\,(q,\theta\,;\,\xi,\kappa) \in T^*(M \times \mathbb{R})\,;\,\kappa > 0\,\} \tag{27}$$

which is the phase space of the homogenized semi-classical Hamiltonian $\mathcal{H}(q,\xi;\theta,\kappa)$. We will now arrive at this manifold more invariantly: Σ is the symplectification of the pre-quantum

$\mathbb{R}$-bundle of T^*M. This point of view will enable us to systematically homogenize symplectic objects in T^*M.

We begin by recalling some basic facts about pre-quantum bundles. Let η $(= \sum pdq)$ be the canonical one-form of T^*M, so that

(28) $$\omega \ = \ -d\eta \ .$$

Then the one-form

(29) $$\alpha \ = \ \eta + d\theta$$

is a connection form with curvature $-\omega$ on the trivial $\mathbb{R}$-bundle

$$P \ := \ T^*M \times \mathbb{R} \ .$$

The $\mathbb{R}$ *bundle with connection* (P, α) *is the pre-quantum bundle of* T^*M. It possesses the following important property. Define a map from $C^\infty(T^*M)$ to vector fields on P, as follows:

(30) $$\begin{array}{rcl} C^\infty(T^*M) & \to & \mathrm{Vect}(T^*M \times \mathbb{R}) \\ H & \mapsto & \Xi^\#_H \ + \ H\partial_\theta \end{array}$$

where $\Xi^\#_H$ is the horizontal lift (with respect to the connection (29)) of the Hamilton vector field of H and ∂_θ is the basic vector field along $\mathbb{R}$.

Proposition 1.1 *(Kostant, Souriau) The map (30) is an injective morphism of Lie algebras, that is*

$$\Theta_{\{H,G\}} \ = \ [\Theta_H \ , \ \Theta_G]$$

where

(31) $$\forall H \in C^\infty(T^*M) \ , \quad \Theta_H \ = \ \Xi^\#_H \ + \ H\partial_\theta \ .$$

Consider, for example, $M = \mathbb{R}^n$. It is well-known that the space of affine Hamiltonians H, that is, of the form

(32) $$H(q,p) \ = \ aq + bp + c \ ,$$

is a $(2n+1)$-dimensional Poisson subalgebra of $C^\infty(\mathbb{R}^{2n})$: it is in fact the Heisenberg Lie algebra. ¿From Proposition 1.1, we know that $\{\Theta_H \ ; \ H \text{ affine } \}$ is then a Heisenberg Lie algebra of vector fields on $P = \mathbb{R}^{2n} \times \mathbb{R}$. This of course is not surprising: P itself is the Heisenberg group and the algebra above is its Lie algebra. The space of homogeneous polynomials on $\mathbb{R}^{2n}$ of degree two is a Lie subalgebra of $C^\infty(\mathbb{R}^{2n})$ isomorphic to the algebra of the group of symplectic linear transformations of $\mathbb{R}^{2n}$. Under Θ, one obtains an $sp(n)$ algebra of vector fields on $P = \mathbb{R}^{n+1}$, generating the action of the symplectic group on the Heisenberg group by automorphisms.

The connection form α makes P a contact manifold. It is well-known that such manifolds have a homogeneous symplectification, which in the present case will turn out to be the manifold Σ of the previous section. The symplectification is the following subset of the cotangent bundle of P, $\Sigma^0 \subset T^*P \setminus \{0\}$:

(33) $$\Sigma^0 \ = \ \{ \ (x, \kappa\alpha_x) \ ; \ x \in P \text{ and } \kappa > 0 \ \} \ .$$

We summarize some basic properties of Σ^0 in the following elementary Lemma:

Lemma 1.2 *Under the natural diffeomorphism,*

$$\begin{array}{rcl} P \times \mathbb{R}^+ & \to & \Sigma^0 \\ (x, \kappa) & \mapsto & (x, \kappa\alpha_x) \end{array}$$

the canonical one-form of T^*P *pulls-back to the form* $\kappa\alpha$ *on* $P \times \mathbb{R}^+$. *Hence:*
(1) Σ^0 *is a symplectic submanifold of* T^*P, *naturally symplectomorphic to* $\Sigma = T^*(M \times \mathbb{R})^+$.

(2) The Hamiltonian

$$\begin{array}{rcl} \kappa : \Sigma^0 & \to & \mathbb{R} \\ (x, \kappa\alpha_x) & \mapsto & \kappa \end{array}$$

generates the $\mathbb{R}$-action induced on Σ^0 by the $\mathbb{R}$ action on P.
(3) For every $c > 0$, the symplectic quotient $\kappa^{-1}(c)/\mathbb{R}$ is naturally symplectomorphic to $(T^*M, c\omega)$.

We will henceforth work with the model $\Sigma = T^*(M \times \mathbb{R})^+$ and will continue to think of P, identified with

$$P = \{ (q, \theta; \xi, \kappa = 1) \in T^*(M \times \mathbb{R})^+ \},$$

as the prequantum line bundle of T^*M, with the connection form $\alpha = \eta + d\theta$.

As we saw in the previous section, a classical Hamiltonian $H(q,p)$ lifts to a Hamiltonian $\mathcal{H}$ on Σ homogeneous of degree one. A general description of this procedure is as follows: Pull-back H to P by the natural projection $\pi : P \to T^*M$, then extend uniquely π^*H to a homogeneous Hamiltonian of degree-one, $\mathcal{H}$, on Σ. It is clear that this description of $\mathcal{H}$ coincides with that of the previous section.

We next consider the problem of homogenizing Lagrangian (or, more generally isotropic) submanifolds of T^*M. Recall that a submanifold $\Lambda_0 \subset T^*M$ is isotropic iff it is flat with respect to the connection on $\pi : P \to T^*M$, that is, if the pull-back to Λ_0 of the symplectic form vanishes. This forces $\dim \Lambda_0 \leq \dim M$, and if equality occurs then Λ_0 is Lagrangian. In the general isotropic case, it makes sense to ask if there is a *global* smooth horizontal section of P over Λ_0. In case Λ_0 is Lagrangian, the image of such a section would be a Legendrian submanifold of P. Global horizontal lifts do not always exist.

Definition 1.3 *We will say that a closed Lagrangian (resp. isotropic) submanifold, $\Lambda_0 \subset T^*M$, is strongly admissible iff there exists a closed conic Lagrangian (resp. isotropic) submanifold $\Lambda \subset \Sigma$ such that*

$$\Lambda_0 = (\Lambda \cap P)/\mathbb{R}. \tag{34}$$

We call Λ a homogenization of Λ_0.

We now investigate when Λ_0 is strongly admissible. Let $\iota : \Lambda_0 \hookrightarrow T^*M$ denote the inclusion of a closed Lagrangian submanifold. Since $0 = \iota^*\omega = -d\iota^*\eta$, the one-form $\iota^*\eta$ is closed. We leave the following as an exercise:

Lemma 1.4 *Λ_0 is strongly admissible iff $\iota^*\eta$ is exact. If $\iota^*\eta = df$ for some $f : \Lambda_0 \to \mathbb{R}$, then*

$$\Lambda = \{ (x, \theta, \kappa) ; \kappa > 0, x \in \Lambda_0 \text{ and } \theta = -f(x) \} \tag{35}$$

is a homogenization of Λ_0.

An example relevant to §§3,4 is the following:

Lemma 1.5 *Let $H \in C^\infty(T^*M)$ and let $\{\phi_t\}$ denote its Hamilton flow. For a given t, let*

$$\Gamma_t^0 = \{ (x, [\phi_t(x)]') ; x \in T^*M \} \subset T^*M \times T^*M = T^*(M \times M)$$

be the twisted graph of the map ϕ_t (prime denotes reflection across the zero section). Then Γ_t^0 is strongly admissible. The twisted graph of the homogenization of H is a homogenization of Γ_t^0. Equivalently, identifying Γ_0^t with T^*M via projection onto the first factor, a homogenization of Γ_t^0 of the form (35) is defined by the function

$$f(x) = \int_0^t \mathcal{L}(\phi_\tau(x))\, d\tau, \tag{36}$$

where $\mathcal{L} : T^*M \to \mathbb{R}$ is the function

$$\mathcal{L} = \partial_r H - H, \tag{37}$$

where $\partial_r = \sum p \frac{\partial}{\partial p}$ is the radial vector field in T^*M.

PROOF The equivalence of both descriptions of a homogenization of Γ_t^0 follows from the equation for $\dot\theta$ in Hamilton's equations for $\mathcal{H}$, namely

$$\dot\theta \;=\; \frac{\partial}{\partial\kappa}\,\kappa\,H(x,\xi/\kappa) \;=\; H(x,\xi/\kappa) - \kappa^{-1}\xi\cdot\nabla_p H(x,\xi/\kappa)\,. \tag{38}$$

(Observe that if $\kappa = 1$ then the right-hand side is $-\mathcal{L}(x,\xi)$.) Therefore we only need to prove that

$$df \;=\; \eta - \phi_t^*(\eta)\,. \tag{39}$$

To prove this for all t we observe that it is true for $t = 0$ and compute the derivative with respect to t of each side. On the right we get (see [28], Proposition 3.6)

$$\phi_t^*(\mathcal{L}_\Xi\eta) \;=\; \phi_t^*\Big(d(\eta(\Xi)) - \omega(\Xi,\cdot)\Big) \;=\; \phi_t^*(d(\eta(\Xi))) - dH\,.$$

On the left, we get

$$\frac{d}{dt}\Big[d(f)_x\Big] \;=\; d\Big[\frac{d}{dt}f\Big]_x \;=\; \phi_t^*\Big(d(\partial_r H)\Big) - dH\,,$$

and since $\partial_r H = \eta(\Xi)$ the result follows.

□

It turns out that many submanifolds of interest (e.g. invariant tori) are *not* strongly admissible; the condition $\iota^*\eta \;=\; df$ is too restrictive. However, there are many cases of interest where

$$\iota^*\eta \;=\; d\log\phi$$

where $\phi : \Lambda_0 \to S^1$. That is, one has $\iota^*\eta \;=\; df$ where f is only defined modulo $2\pi\mathbb{Z}$. Then the previous constructions can be carried out if we work on a periodic version of P, that is, if we take $P = T^*M \times S^1$ so that θ is now 2π-periodic. (In the language of cohomology, strong admissibility amounts to $[\iota^*\eta] = 0$ in $H^1(\Lambda_0,\mathbb{R})$ while the weaker version requires that the cohomology class of $\iota^*\eta$ in $H^1(\Lambda_0, S^1)$ vanishes.) Clearly there's nothing special about the number 2π; we formulate the results in general:

Definition 1.6 *Given $\hbar_0 > 0$, let $S^1_{\hbar_0} \;=\; \mathbb{R}/(2\pi/\hbar_0)\,\mathbb{Z}$ and*

$$P_{\hbar_0} \;=\; T^*M \times S^1_{\hbar_0}\,,$$

$$\Sigma_{\hbar_0} \subset T^*P_{\hbar_0}$$

be the obvious periodic variants of P, Σ. We will say that $\Gamma_0 \subset T^*M$ is $\hbar_0$-admissible iff there exists a closed conic Lagrangian submanifold, $\Lambda \subset \Sigma_{\hbar_0}$ such that (34) holds.

This is a geometrical version of the Bohr-Sommerfeld condition.

Lemma 1.7 *Λ_0 is $\hbar_0$-admissible iff there exists $\phi : \Lambda_0 \to S^1_{\hbar_0}$ such that $\iota^*\eta \;=\; d\log\phi$. In that case,*

$$\Lambda \;=\; \{\,(x\;,\;e^{i\theta}\,,\kappa)\;;\;\kappa > 0\;,\;x\in\Lambda_0 \text{ and } e^{i\theta} \;=\; \phi(x)\,\}$$

is a closed conic Lagrangian submanifold of Σ satisfying (34).

Remarks:

1.- Obviously a strongly admissible Λ_0 is $\hbar_0$ admissible for all $\hbar_0$.

2.- In semi-classical asymptotics associated with $\hbar_0$-admissible objects, it is known that one has a nice theory if the values of $\hbar$ are restricted to go to zero along the sequence of values

$$\hbar \;=\; \frac{\hbar_0}{k}\;,\; k = 1, 2, \cdots\;.$$

We see here a geometric interpretation of this fact: the values above are the reciprocals of the eigenvalues of D_θ.

3.- For ease of notation, we will say that Λ_0 is *admissible* if it is 1-admissible, leaving to the reader the task of rescaling to obtain the general $\hbar_0$-admissible case.

2 Semi-Classical States

In this section we study the relationship between the notion of compound asymptotics, as developed for example in Chapter 7 of [17], and the $\hbar$-transform, which we define as the Fourier transform in κ. We will restrict our attention in this section to compact admissible Lagrangians and the 'periodic' version of P, with structure group S^1. Therefore the semi-classical homogenization of T^*M is

$$\Sigma = T^*(M \times S^1)^+$$

quantized by $L^2(M \times S^1)$.

2.1 Definitions and some elementary results.

We begin by defining a very general concept of *semi-classical family* of wave functions on a manifold M. We keep the notation of the previous section: we denote by Σ the open set in $T^*(M \times S^1) \setminus \{0\}$ defined by:

$$\Sigma \,:\, \kappa > 0$$

where κ is the variable dual to the circular variable θ.

Definition 2.1 *Let M be a smooth manifold, and $\{\psi_m\}$ a sequence of smooth half-densities on M. We will say that $\{\psi_m\}$ is a* semi-classical family *(scf) iff the series*

$$\Psi \;=\; \sum_{m=1}^{\infty} \psi_m(x)\, e^{im\theta} \tag{40}$$

converges weakly to a distribution Ψ on $M \times S^1$, and

$$WF(\Psi) \;\subset\; \Sigma\,. \tag{41}$$

We will say that Ψ is the $\hbar$-transform of the family.

Remark: If one has a distributional half-density, Ψ, on $M \times S^1$ satisfying (41), then its Fourier coefficients are automatically smooth. This is because the m-th Fourier coefficient of Ψ is the push-forward

$$\psi_m \;=\; \frac{1}{2\pi}\,\pi_*\,\left(e^{-im\theta}\,\Psi\right)$$

where $\pi : M \times S^1 \to M$ is the natural projection, and condition (41) ensures that no covectors in the wave-front set of Ψ are conormal to the fibers of π. Hence there is no loss of generality in the definition above in assuming that the ψ_m are smooth.

Lemma 2.2 *A sequence $\{\psi_m\}$ of smooth half-densities on M is a scf if for every compact $K \subset M$ contained in a coordinate chart U, $(x_1, \dots x_n)$ and every multi-index α there exists a constant $C_{K,\alpha}$ such that*

$$\sup_{x\in K}\, \frac{1}{m^{|\alpha|}}\, |\, D_x^\alpha\, \psi_m(x)\,| \;\leq\; C_{K,\alpha}\,. \tag{42}$$

Before presenting the proof, a couple of remarks. Implicitly in (42) is the identification of half-densities and functions on U provided by the coordinate functions. Notice that as a corollary we get that any expression of the sort arising in WKB theory, that is

$$\psi_m(x) \;=\; a(x,m)\, e^{imS(x)} \tag{43}$$

where a has symbolic behavior on m, defines a semi-classical family.
Proof of the Lemma: Condition (42) with $\alpha = 0$ says that ψ_m is bounded on compact sets uniformly on m. This implies that the series (40) converges weakly: if $u(x,\theta)$ is a test function on $M \times S^1$, then

$$\left| \int_0^{2\pi} e^{im\theta}\, u(x,\theta)\; d\theta \right| \;\leq\; \frac{2}{m^2}\, \sup\, \left(D_\theta^2\, u\right)\;,$$

which shows that the series paired against u converges and is bounded by the C^2 norm of u.

Working locally in some coordinates $(x_1,\ldots,x_n,\theta)$ take now a point $(x^0,\theta^0,\xi^0,\kappa^0)$. To see if it is not in WF (Ψ), we consider the large positive λ behavior of the pairing

$$I(\lambda) \;=\; \left(\rho_1(\theta)\,\rho_2(x)\,\Psi\;,\;e^{i\lambda\,(x\xi+\theta\kappa)}\right)$$

where $\rho_1(\theta)\,\rho_2(x)$ are smooth cut-off functions non vanishing at (x^0,θ^0). Clearly,

$$I(\lambda) \;=\; \sum_{m=1}^{\infty} \hat{\rho}_1(\lambda\kappa-m)\;\widehat{\rho_2\psi_m}(\lambda\xi)\;. \tag{44}$$

We must show that the estimates (42) imply that this is $O(\lambda^{-N})$ for each $N>1$, uniformly in (ξ,κ) in a neighborhood of (ξ^0,κ^0). In fact, it suffices to take ξ of Euclidean norm one:

$$\|\,\xi\,\| \;=\; 1\;, \tag{45}$$

a fact that will simplify the writing below.

Since $\rho_2\in C_0^\infty$, for every $K>0$ there exists $A_K>0$ such that

$$|\,\hat{\rho}_1(\mu)\,| \;\le\; \frac{A_K}{(1+|\mu|)^K}\;.$$

It follows that

$$\forall\,\lambda>0\;,\;\;\kappa<0\quad |\,\hat{\rho}_1(\lambda\kappa-m)\,| \;\le\; \frac{A_K}{(1+m)^K}\;.$$

Hence

$$|\,I(\lambda)\,| \;\le\; A_K\sum_{m=1}^{\infty}\frac{1}{(1+m)^K}\left|\,\widehat{\rho_2\psi_m}(\lambda\xi)\,\right|\;. \tag{46}$$

On the other hand, by assumption (45), we have that

$$\lambda^{2N}\,\hat{f}(\lambda\xi) \;=\; (\widehat{\Delta^N f})\,(\lambda\xi)$$

where Δ is the Euclidean Laplacian, this for any $f\in C_0^\infty$. It follows that

$$\lambda^{2N}\left|\hat{f}(\lambda\xi)\right| \;\le\; \int_{\mathbb{R}^n}\left|\Delta^N f\right|(x)\,dx \;\le\; \mathrm{Vol}\,(\mathrm{supp}\,f)\;\sup|f(x)|\;. \tag{47}$$

Apply this inequality with $f=\rho_2\psi_m$, using the fact that

$$\sup\left|\Delta^N\rho_2\psi_m\right| \;\le\; C_N\,m^{2N}\;.$$

Hence we get that

$$\lambda^{2N}\left|\,\widehat{\rho_2\psi_m}(\lambda\xi)\,\right| \;\le\; B_N\;m^{2N}\;,$$

for some constant B_N. Multiplying (46) by λ^{2N} and taking $K=2N+2$ we see that $I(\lambda)$ is $O(\lambda^{-2N})$. □

It would be desirable to have a converse to this lemma, or otherwise establish local criteria on $\{\psi_m\}$ on M to be a scf. A moment's thought however shows that this is subtle: estimates of the type (42) are unchanged if we multiply ψ_m by a phase factor $e^{i\omega_m}$ with an m-dependent phase. Such phase factors however can be expected to change significantly the $\hbar$-transform of the family. We will see in the next subsection how to choose the phase of a family $\{\psi_m\}$ in a "coherent" fashion.

Attached to any semi-classical family is its *frequency set*, FS($\{\psi_m\}$), which we define next. For simplicity we state the definition in the case $M=\mathbb{R}^n$, referring the reader to [17],Chapter 7 Proposition 2.2 for the proof that the local definition below extends to manifolds, the frequency set of a semi-classical family being an invariantly-defined closed set of the cotangent bundle T^*M (possibly intersecting the zero section).

Definition 2.3 *(see also [35], Definition IV-7.) The frequency set of a semi-classical family, $\{\psi_m\}$, on $\mathbb{R}^n$ is defined by the following condition: $(q^0, p^0) \in \mathbb{R}^{2n}$ is* not *in $FS(\{\psi_m\})$ iff there exist a cut-off function, $\rho \in C_0^\infty(\mathbb{R}^n)$ and a neighborhood V of p in $\mathbb{R}^n$ such that $\rho(q^0) \neq 0$ and $\forall N > 0\ \exists C_N > 0$ such that*

$$\forall p \in V \qquad \left| \widehat{\rho\psi_m}\,(mp) \right| \ \leq\ \frac{C_N}{m^N}\ .$$

As we will prove below, there is a close relationship between the frequency set of a scf and the wave-front set of its $\hbar$-transform. The result is as follows. Identify P with the submanifold of Σ where $\kappa = 1$:

$$P\ =\ \{\ (x, \xi; \theta, \kappa = 1)\ \}$$

Proposition 2.4 *Let $\{\psi_m\}$ be a semi-classical family on a manifold M, and let Ψ be its $\hbar$-transform. Then the projection of the intersection of the wave-front set of Ψ with P contains the frequency set of $\{\psi_m\}$:*

$$FS(\{\psi_m\}) \subset \pi\ (\ WF(\Psi) \cap P\ )\ .$$

To prove this proposition we will need to use the $\hbar$-transform of the asymptotic Fourier transforms. We now digress to define it.

Definition 2.5 *If $u \in C_0^\infty(\mathbb{R}^n \times S^1)$, define*

$$\mathcal{F}(u)(p,s)\ =\ \int_{\mathbb{R}^n} u(x\,,\ s - p\cdot x)\ dx\ .$$

If we decompose u in its Fourier coefficients,

$$u(x,\theta)\ =\ \sum_m\ u_m(x)\, e^{im\theta}\ ,$$

then

$$\mathcal{F}(u)(p,s)\ =\ \sum_m\ \hat{u}_m\,(mp)\, e^{ims}\ .$$

The following is an easy exercise:

Lemma 2.6 *The operator $\mathcal{F}$ is an elliptic Fourier integral operator associated to the canonical relation*

(48) $$\{\ (q, \sigma p\,;\, \theta, \sigma\,;\, p, \sigma q\,;\, s, \sigma)\ ;\ s = \theta + qp\,,\ \sigma \neq 0\ \}\ .$$

Proof of the Proposition. Since the statement is local, we can assume M is an open set in $\mathbb{R}^n$. By ellipticity of $\mathcal{F}$, the wave-front set of $\mathcal{F}\,(\Psi)$ is the image of WF (Ψ) under the canonical relation (48).

Let (q^0, p^0) be a point in the complement of π (WF $(\Psi) \cap P$). We will prove that it is *not* in the frequency set of $\{\psi_m\}$. The assumption implies that there exist: a cut-off function $\rho(q)$ such that $\rho(q^0) \neq 0$ and a neighborhood V containing p^0 such that

(49) $$\forall\ \theta\ ,\ p \in V\ ,\ q \in \mathbb{R}^n \quad (q, p;\ \theta, 1) \notin \mathrm{WF}\,(\rho\Psi)\ .$$

By (48), it follows that WF $(\mathcal{F}\,(\rho\Psi))$ must be empty: on the one hand, by (49) it must be included in $\{\ \sigma\ =\ 0\}$ but since by assumption WF $(\rho\Psi) \subset \Sigma$, again by (48) WF $(\mathcal{F}\,(\rho\Psi))$ is disjoint from this set. Hence $\mathcal{F}\,(\rho\Psi)$ is *smooth* On the other hand, it is easy to see that

$$\mathcal{F}\,(\Psi)\,(p,s)\ =\ \sum_{m=1}^{\infty}\ \widehat{\rho\psi}_m\,(mp)\, e^{ims}\ .$$

Hence the coefficients $\hat{\psi}_m\,(mp)$ are rapidly decreasing in m, uniformly in p in a perhaps smaller neighborhood V. □

The proof of the previous proposition actually includes a characterization of the projection of the wave front set of the $\hbar$-transform of a scf:

Corollary 2.7 *With the previous notations, (q^0, p^0) is not in the projection of $WF(\Psi) \cap P$ iff there exist a cut-off function ρ with $\rho(q^0) \neq 0$ and a neighborhood V of p^0 such that*

$$\forall\, N > 0\,,\ \alpha \quad \exists C > 0 \quad \forall\, p \in V\,, \qquad \left| D^\alpha\, \widehat{\rho\psi_m}\,(mp) \right| \leq \frac{C}{m^N}\,.$$

Definition 2.8 *The semi-classical wave-front set of $\{\psi_m\}$ is defined to be the set of the previous corollary, that is, the projection of $WF(\Psi) \cap P$ to T^*M. It will be denoted $SWF\{\psi_m\}$.*

Thus the SWF of a scf is a finer invariant than the frequency set of the family: WF (Ψ) contains information on the phases of the ψ_m, while the frequency set only pertains to their size.

2.2 Lagrangian semi-classical states.

Definition 2.9 *Let $\Lambda_0 \subset T^*M$ be an admissible Lagrangian submanifold. A* Lagrangian semi-classical state *(scs) associated with Λ_0 is a sequence $\{\psi_m\}$ of (square integrable) smooth half-densities on M such that its $\hbar$-transform,*

$$\Psi \;=\; \sum_{m=1}^{\infty}\ \psi_m\, e^{im\theta}$$

is a classical Lagrangian distribution associated to a horizontal lift of Λ_0,

$$\Psi \in I^l\,(M \times S^1\ ,\ \Lambda)\ , \quad \Lambda \subset \Sigma\ .$$

Notice that, in particular, a scs is a semi-classical family; of course one of a very special kind. We will see in fact that a scs is in particular an oscillatory integral of the type considered by Duistermaat, [13], or a *compound asymptotic* in the terminology of Guillemin and Sternberg, [17]. For convenience, we recall the local definition: locally a sequence $\{\psi_m\}$ is a compound asymptotic or a classical oscillatory function associated with a Lagrangian $\Lambda_0 \subset T^*M$ iff it is of the form

$$\psi_m\,(x) \;=\; \int\ e^{im\phi_0\,(x,w)}\ a(x,w,m)\ dw \tag{50}$$

where ϕ_0 is a non-degenerate phase function parametrizing Λ_0 and $a(x;w,\mu)$ is a classical symbol:

$$a(x;w,\mu)\ \sim\ \sum_{j=0}^{\infty}\ a_j(x,w)\ \mu^{l-j}$$

in C^∞ as $\mu \to \infty$. (The symbolic estimates on a are uniform on (x,w) in compact sets.) The point we wish to make in this section is that *by the $\hbar$-transform, the theory of compound asymptotics reduces to the standard theory of Lagrangian distributions.* We will derive a local expression for a scs, and observe that it is identical to that of a compound asymptotic. Before starting in that direction, we first notice that scs's are invariant under multiplication/division by m, which corresponds, on the $\hbar$-transform side, to differentiation/integration with respect to the variable θ:

Lemma 2.10 *If $\{\psi_m\}$ is a scs, so are $\{\,m\psi_m\,\}$ and $\{\,m^{-1}\psi_m\,\}$. The latter are associated to the same Lagrangian $\Lambda \subset \Sigma$ as $\{\psi_m\}$.*

PROOF If Ψ is a Lagrangian distribution associated to a *closed* Lagrangian $\Lambda \subset \Sigma$, then so is $D_\theta\Psi$, which gives that $\{\,m\psi_m\,\}$ is a scs. To see that

$$\sum_{m=1}^{\infty}\ \frac{1}{m}\ \psi_m(x)\ e^{im\theta}$$

is Lagrangian, we must use the fact that the obvious relative parametrix of D_θ is a pseudodifferential operator associated to a pair of intersecting Lagrangians: the diagonal in $[T^*(M \times S^1) \setminus$

$0] \times [T^*(M \times S^1) \setminus 0]$ and the flow-out of $\{ \kappa = 0 \}$, see [20]. Since Λ by assumption does *not* intersect $\{ \kappa = 0 \}$, the action of this operator on Ψ is identical to that of a ΨDO of order (-1).

□

REMARK: The fact that the relative parametrix of D_θ acts on semi-classical families as a pseudodifferential operator of order (-1) is fundamental for our approach to semi-classical problems, and we will make extensive use of this fact.

We will now prove the equivalence of scs and compound asymptotics.

Lemma 2.11 *Let $\phi_0(x;w) \in C^\infty(U \times W)$, $U \subset \mathbb{R}^n$ and $W \subset \mathbb{R}^N$ open, be a non-degenerate phase function parametrizing an admissible Λ_0. Then the phase*

$$\phi(x,\theta\,;\,w,\kappa) \;=\; \kappa\,(\theta + \phi_0(x,w)) \tag{51}$$

is a non-degenerate phase function parametrizing a horizontal lift of Λ. Here $(w,\kappa) \in W \times \mathbb{R}^+$.

PROOF Consider the set C_ϕ defined by the equations $\partial_\kappa \phi = 0$, $\partial_w \phi = 0$. Clearly

$$C_\phi \;=\; \{\; (x,\theta\,;\,\kappa,w) \;;\; \theta \;=\; -\phi_0(x,w) \text{ and } \partial_w\phi_0 \;=\; 0 \;\} \;. \tag{52}$$

It is obvious that the ϕ is non-degenerate if ϕ_0 is, and that the Lagrangian submanifold parametrized by ϕ is

$$\Lambda \;=\; \{\; (x,-\phi_0(x,w)\;;\;\kappa\partial_w\phi_0(x,w),\kappa) \;;\; \partial_w(x,w) = 0 \;\kappa > 0 \;\} \;. \tag{53}$$

If one here sets $\kappa = 1$ and divides by the action of S^1, one obtains the Lagrangian parametrized by ϕ_0. This is sufficient to prove the lemma. We would like however to point out explicitly that the rule

$$C_{\phi_0} \ni \theta \;\mapsto\; \phi_0(x,w)$$

(where $C_{\phi_0} = \{(x,w) \;;\; \partial_w\phi_0(x,w) = 0\}$) defines a function f on C_{ϕ_0} such that

$$df \;=\; \iota^*(xdp)\;, \tag{54}$$

where $\iota(x,w) \;=\; (x,(d_x\phi_0)_{(x,w)})$ is the map parametrizing Λ_0 and xdp is the canonical one-form of T^*M. Equation (54), which we leave as an easy exercise, implies that on a horizontal lift of Λ_0, $\theta = \theta_0 - \phi_0(x,w)$, which is satisfied by points on Λ by (53).

□

Proposition 2.12 *$\{\psi_m\}$ is a Lagrangian scs associated with Λ_0 iff it is a compound asymptotics, that is iff it can be written locally in the form (50).*

PROOF Assume $\{\psi_m\}$ is a Lagrangian scs. By Lemma 2.11, the $\hbar$-transform of $\{\psi_m\}$ is given locally by an oscillatory integral of the form

$$\Psi\,(x,\theta) \;=\; \int e^{i\kappa\,(\theta+\phi_0(x,w))}\; b(x,\theta\,;\,w,\kappa)\; dw\; d\kappa\;, \tag{55}$$

where b is a classical symbol compactly supported in (x,θ,w). Taking the m-th Fourier coefficient of this, we find that ψ_m can be written locally as

$$\int e^{i\kappa\phi_0(x,w)}\;\tilde{b}\,(x,m-\kappa\,;\,w,\kappa)\; dw\; d\kappa\,,$$

where $\tilde{b}$ is the Fourier transform of b in the θ variable:

$$\tilde{b}\,(x,\mu\,;\,w,\kappa) \;=\; \frac{1}{2\pi}\int_0^{2\pi} e^{-i\mu\,\theta}\; b(x,\theta\,;\,w,\kappa)\; d\theta\;.$$

(Without loss of generality we can take b with small support in (x, θ), and hence in the previous integral we might as well integrate over the real line.) Substituting κ by $m-\kappa$, we obtain (50) with

$$a(x, w, m) \;=\; \int e^{-i\kappa\phi_0(x,w)}\; \tilde{b}\,(x, \kappa\,;\, w, m-\kappa)\; d\kappa\;. \tag{56}$$

Our task is to show that this is a symbol, as indicated. Since b is a classical symbol, by assumption, we have an asymptotic expansion

$$b(x, \theta\;,\; w, \kappa) \sim \sum_{j=0}^{\infty} b_j(x, \theta; w)\; \kappa^{d-j}\;, \tag{57}$$

as $\kappa \to \infty$. It is clear that a completely analogous expansion holds for the Fourier transform of b in the θ variable. Hence

$$a(x, w, m) \;\sim\; \sum_{j=0}^{\infty} \int e^{-i\kappa\phi_0(x,w)}\; \tilde{b}_j\,(x, \kappa\,;\, w)(m-\kappa)^{d-j}\; d\kappa\;,$$

which by the inversion of the Fourier transform gives

$$a(x, w, m) \;\sim\; \sum_{j=0}^{\infty} \left(\, (m - D_\theta)^{d-j}\; b_j\,\right)\; (x\;,\; -\phi_0(x, w)\;,\; w)\;. \tag{58}$$

Conversely, take an oscillatory integral of the form (50). Assume first that the amplitude a is independent of m. Then (by summing a geometric series) the $\hbar$-transform of $\{\psi_m\}$ is

$$\Psi\,(x, \theta) \;=\; \int \frac{a(x, w)}{1 - e^{i[\theta + \phi_0(x,w)]}}\; dw\;. \tag{59}$$

The function

$$\frac{a(x, w)}{1 - e^{[i\theta + \phi_0(x,w)]}}$$

represents a distribution in (x, θ, w)-space conormal to the hypersurface $\theta = i\phi_0(x, w)$, and (59) shows that Ψ is the push-forward of it to (x, θ) space. By the assumption that ϕ_0 is non-degenerate, this shows that Ψ is a Lagrangian distribution associated to

$$\Lambda \;=\; \{\; (x, \theta\,;\, \kappa p, \kappa\,;\; \exists w\;\, \theta = -\phi_0(x, w)\;,\; \partial_w\phi_0(x, w)\;,\; p = \partial_x\phi_0(x, w)\;\}\;,$$

which is precisely a horizontal lift of Λ_0. The general case (i.e. when a depends symbolically on m) is an asymptotic sum of derivatives and integrals (with respect to θ) of the previous case. Since these operations preserve the class of scs, see Lemma 2.10, the proof is finished.

$\square$

Finally, we note that Lagrangian scs's obviously have a symbol:

Definition 2.13 *The symbol of a scs $\{\psi_m\}$ is defined as the symbol of its $\hbar$-transform, Ψ.*

2.3 Hermitian semi-classical states

In this section we will construct semi-classical families associated to admissible isotropic submanifolds, $\Gamma_0 \subset T^*Q$, generalizing the construction of Lagrangian semi-classical states of §2.2. Our construction is similar in spirit to that of Ralston, [34], and Colin de Verdière, [6], with the difference that a symbol calculus (albeit a complicated one) exits in the present case.

Let M be a smooth manifold, and $\Gamma \subset T^*M \setminus \{0\}$ a closed conic isotropic submanifold. In [16], [1] Boutet de Monvel and Guillemin define classes of distributions on M, $I^p(M, \Gamma)$, with wave-front set contained in Γ and generalizing the concept of Lagrangian distributions. The elements of $I^p(M, \Gamma)$ are called Hermite distributions associated to Γ.

Definition 2.14 *A family $\{\psi_m\}$ in $L^2(Q)$ is a Hermite s.c state associated to an admissible $\Gamma_0 \subset T^*Q$ iff*

$$\Psi \; = \; \sum_{m=1}^{\infty} \psi_m(x) \; e^{im\theta}$$

converges weakly to a Hermite distribution on $Q \times S^1$ associated to a horizontal lift of Γ_0.

Our treatment of Hermite families will be very brief. We will simply indicate the local nature of the Hermitian states and give some examples. It turns out that coherent states at a point, or wave-packets, form a Hermite family. In the next section we will use this fact, together with the invariance of the class of Hermite distributions under Fourier integral operators, to derive a theorem of propagation of wave packets similar to those of Cordoba-Fefferman, [9], and Hagedorn, [22].

We begin by discussing the local expressions of Hermite distributions. For all that follows we refer the reader to the source, [1]. Let $\Gamma \subset T^*U \setminus \{0\}$, $U \subset \mathbb{R}^m$ open, be a closed isotropic submanifold of dimension $n-l$. Let $\phi(x,w) \in C^\infty(U \times W)$ with $W \subset \mathbb{R}^N$ open be a smooth phase function. Hence the critical set

$$C_\phi \; = \; \{ \; (x,w) \; ; \; d_w\phi \; = \; 0 \; \} \tag{60}$$

is a smooth manifold and the map

$$\begin{array}{ccc} C_\phi & \to & T^*U \setminus \{0\} \\ (x,w) & \mapsto & (x, d_x\phi) \end{array} \tag{61}$$

is a Lagrangian immersion, which, since we are working locally, will be assumed to be an embedding. To parametrize Γ, split the w variables in two sets,

$$w \; = \; (\tau \, , \, \eta) \; \in \; \mathbb{R}^{N-l} \times \mathbb{R}^l \; . \tag{62}$$

Definition 2.15 *We say that ϕ is a non-degenerate function parametrizing Γ iff:*
(a) C_ϕ intersects transversely the set

$$\Omega \; := \; \{ \; \eta \; = \; 0 \; \} \; , \; \textit{and}$$

(b) The embedding (61) maps $C_\phi \cap \Omega$ onto Γ.

Let us now assume that Γ and W are conic, and ϕ is positive homogeneous of degree one in w. Keeping the notations of the definition, Hermite distributions on U associated with Γ are given by oscillatory integrals of the form

$$\int e^{i\phi(x,\omega)} \; a\left(x, \tau, \frac{\eta}{\sqrt{|\tau|}}\right) \; d\tau \, d\eta \tag{63}$$

where $a(x,\tau,\eta)$ has symbolic behavior on τ and is rapidly decreasing in η. A bit more precisely, a satisfies estimates of the form

$$| \; D_x^\alpha \, D_\tau^\beta \, D_\eta^\gamma \; a(x,\tau,\eta)| \leq C \; |\tau|^{m-|\gamma|} \; (1+|\eta|)^{-r} \tag{64}$$

on every compact $K \subset\subset U$ and for all $r > 0$ and multiindices $\alpha \, , \, \beta \, , \, \gamma$. It is not hard to see that the wave-front set of (63) is contained in Γ: by rapid decrease in η, the amplitude

$$a\left(x, \tau, \frac{\eta}{\sqrt{|\tau|}}\right)$$

is rapidly decreasing uniformly in cones in (τ, η)-space with closure contained in the complement of Ω. We will denote the space of such symbols by $\mathfrak{H}^m(n-l, l)$.

We now turn to Hermitian semi-classical families. Let $\Gamma_0 \subset T^*Q$ be an admissible isotropic submanifold.

Proposition 2.16 *A family $\{\psi_m\}$ is a Hermitian semi-classical state associated with Γ_0 iff it can locally be written in the form*

$$\{\psi_m\}(x) \;=\; \int e^{im\phi_0(x,\eta)}\; a\left(x, m, \frac{\eta}{\sqrt{m}}\right)\, d\eta \tag{65}$$

where ϕ_0 is a non-degenerate phase function parametrizing an open subset of Γ_0, and

$$a(x,m,\eta) \;\sim\; \sum_{j=0}^{\infty} a_j(x,\eta)\, m^{l-j/2}$$

where $\forall j \;\; a_j \in \mathfrak{H}^j(n-l,l)$.

PROOF By the theorem of equivalence of phase functions of [1], all we need to notice is that the phase function

$$\phi(x,\theta;\eta,\kappa) \;=\; \kappa\,(\theta + \phi_0(x,\eta))$$

is a non-degenerate phase function parametrizing a horizontal lift of Γ_0. The rest of the proof is identical to that of Proposition 2.12.

□

We recall that the symbol of an Hermite distribution is a symplectic spinor on the associated isotropic. By [1] the symbol of an Hermitian scs can be identified with a symplectic spinor on the isotropic $\Gamma_0 \subset T^*M$. We make this explicit in the following case:

Example: Wave packets. The simplest co-isotropic is of course a single point, $\Gamma_0 = \{(x_0, \xi_0)\}$.

Definition 2.17 *A generalized wave packet centered at $(x_0,\xi_0) \in T^*M$ is a Hermitian semi-classical state associated with $\Gamma_0 = \{\,(x^0,\xi^0)\,\}$.*

As we will see (Lemma 2.20 below), the standard wave packets (or coherent states) in $\mathbb{R}^n$ are a particular case of Hermitian scs. In [33] we estimate the matrix elements between eigenfunctions of a Hamiltonian and wave packets.

Specializing (65), we see that a wave packet can be written in local coordinates in the form

$$\psi_m(x) \;=\; e^{im[(x-x_0)\cdot\xi_0+\theta_0]} \int e^{im(x-x_0)\cdot\eta}\, a(x,m,\frac{\eta}{\sqrt{m}})\, d\eta\,. \tag{66}$$

if we lift the point (x_0,ξ_0) to (x_0,ξ_0,θ_0).

Turning to the symbol of a wave packet, a symplectic spinor on $\{(x_0,\xi_0)\}$ is simply a smooth vector in the metaplectic representation of the symplectic group of $W := T_{(x_0,\xi_0)}(T^*M)$. If we introduce a Riemannian metric on the manifold M, we get a direct sum decomposition $W = V \oplus H$, where $V \cong T^*_{x_0}M$ is the kernel of the cotangent fibration and H the horizontal subspace. Both V and H are Lagrangian subspaces; therefore (see [29] §1.2.5) there is a natural realization of the metaplectic representation of $\mathrm{Mp}(W)$ in $L^2(T^*_{x_0}M)$. *Therefore the symbol of a wave packet centered at (x_0,ξ_0) is a Schwartz function on $T^*_{x_0}M$.* The following definition is therefore natural. We mention that, independently and simultaneously, Karasev and Vorobjev have arrived at a similar concept, see [27] §2v.

Definition 2.18 *A Gaussian wave packet is a Hermitian scs whose symbol is a Gaussian.*

Observe that in the representation (66), the parametrizing map

$$\begin{array}{rcl} C_{\phi_0} = \{(x_0,\eta)\} & \to & T^*M \\ (x_0,\eta) & \mapsto & (x_0,\xi_0+\eta) \end{array} \tag{67}$$

identifies the space of the η variables with $T^*_{x_0}M$.

Lemma 2.19 *Under (67), the symbol of the Hermitian scs (66) is the Schwartz function* $\eta \mapsto a_0(x_0, \eta)$.

The proof follows from the definition of the symbol of an Hermite distribution given by an oscillatory integral representation, [1].

Let $\{\psi_m\}$ be a Gaussian wave packet centered at (x_0, ξ_0), and introduce local coordinates near x_0. Then ψ_m is given by an expression of the form (66) where, by hypotheses, $a_0(x_0, \eta)$ is a Gaussian in η, that is

$$a_0(x_0, \eta) \;=\; e^{-\eta \cdot A\eta/2}\,,$$

where A is a positive definite symmetric matrix. Modeling on the case of $\mathbb{R}^n$, let us pick

$$\theta_0 \;=\; \frac{1}{2}\, x_0 \cdot \xi_0\,,$$

a choice dictated by Heisenberg group considerations that we won't go into.

Lemma 2.20 *There exists* $\rho \in C_0^\infty$ *such that* $\rho(x_0) = 1$ *and*

$$\psi_m \;=\; (2\pi)^{n/2}\, |A|^{-1/2}\, \rho(x)\, e^{im[x\cdot\xi_0 - x_0\cdot\xi_0/2]}\, e^{-m(x-x_0)\cdot A^{-1}(x-x_0)/2} + O(m^{l-1/2}).$$

PROOF Write

$$a_0(x, \eta) \;=\; a_0(x_0, \eta) + \sum_{j=1}^{n} (x - x_0)_j\, b_j(x, \eta)\,,$$

where $(x - x_0)_j$ is the jth coordinate of $x - x_0$. This can be done in a neighborhood of x_0. Let ρ have support in that neighborhood and satisfy $\rho(x_0) = 1$. We must estimate the integrals

$$I_j(x, m) \;=\; \int e^{im(x-x_0)\cdot\eta}\, \rho(x)\, (x - x_0)_j\, b_j(x, \eta/\sqrt{m})\, d\eta\,.$$

We integrate by parts: Since $D_{\eta_j} e^{im(x-x_0)\cdot\eta} = m(x - x_0)_j e^{im(x-x_0)\cdot\eta}$,

$$I_j(x, m) \;=\; \frac{-1}{m^{3/2}} \int e^{im(x-x_0)\cdot\eta}\, \rho(x)\, (D_{\eta_j} b_j)(x, \eta/\sqrt{m})\, d\eta\,,$$

and the integral is easily seen to be $O(1)$, uniformly on x near x_0.

□

3 Semi-Classical Fourier Integral Operators

We now discuss the operators whose Schwartz kernels are semi-classical states associated to non-compact Lagrangians. We begin with a preliminary remark:

Lemma 3.1 *Let* M_1 *and* M_2 *be manifolds, and*

$$\mathcal{F} \,:\, C^\infty(M_1 \times S^1) \to C^\infty(M_2 \times S^1)$$

an operator. Then $\mathcal{F}$ *intertwines the* S^1 *actions iff its Schwartz kernel is the pull-back by the map*

$$\begin{array}{rccc} \pi \,: & M_2 \times S^1 \times M_1 \times S^1 & \to & M_2 \times M_1 \times S^1 \\ & (x_2, e^{i\theta_2}, x_1, e^{i\theta_1}) & \mapsto & (x_2, x_1, e^{i(\theta_1 - \theta_2)}) \end{array}$$

of a distribution $\mathcal{F}_0$ *on* $M_2 \times M_1 \times S^1$. *If this is the case,* $\mathcal{F}$ *is a Fourier integral operator associated to the canonical relation* $\overline{\Gamma} \subset T^*(M_1 \times S^1 \times M_2 \times S^1)$ *iff* $\mathcal{F}_0$ *is a Lagrangian distribution associated to the Lagrangian submanifold*

(68) $$\Lambda \;=\; \{\, (x_2, x_1, e^{i\theta}; \xi_2, \xi_1, \kappa)\,;\, (x_2, e^{i\theta}, x_1, 1, \xi_2, \kappa, -\xi_1, \kappa) \in \overline{\Gamma}\,\}\,.$$

PROOF Part one of the lemma follows from the fact that the operator $\mathcal{F}$ intertwines the S^1 actions iff its Schwartz kernel is annihilated by the vector field $\frac{\partial}{\partial\theta_1}+\frac{\partial}{\partial\theta_2}$. ¿From this it also follows that its wave-front set is contained in $\{\kappa_1=-\kappa_2\}$. We leave the rest of the proof as an exercise (introduce local coordinates $\theta_1-\theta_2$ and $\theta_1+\theta_2$).

□

We will usually identify the Schwartz kernel of an operator $\mathcal{F}$ that intertwines the S^1 actions with the distribution $\mathcal{F}_0$ of the Lemma.

Let $\Gamma\subset T^*M_1\times T^*M_2$ be a canonical relation. Recall the notation: Γ' is the set of all $(x_1,p_1;x_2,p_2)$ such that $(x_1,p_1;x_2,-p_2)\in\Gamma$. By definition Γ is a canonical relation iff Γ' is a Lagrangian submanifold of $T^*M_1\times T^*M_2$.

Definition 3.2 *(a) A canonical relation $\Gamma\subset T^*M_1\times T^*M_2$ will be called admissible iff Γ' is admissible in the sense of §1.2. (b) If $\Gamma\subset T^*M_1\times T^*M_2$ is an admissible canonical relation, a sequence of operators $\{F_k\}$,*

$$F_k\,:C^\infty(M_1)\to C^\infty(M_2)\quad k=1,2,\ldots$$

will be called a semi-classical Fourier integral operator (scFIO) from M_1 to M_2 iff the $\hbar$-transform ($\hbar=1/k$) of the Schwartz kernels of the F_k is a Lagrangian scs associated with a horizontal lifting of Γ'.

Notice that, by Lemma 3.1, if $\{F_k\}$ is a scFIO then the operator $\mathcal{F}$ from $M_1\times S^1$ to $M_2\times S^1$ which is defined by $\mathcal{F}|_{D_{\theta_1}=k=D_{\theta_2}}=F_k$ is an ordinary Fourier Integral Operator. Our main example will be the approximation to the propagator for a Schrödinger-type operator that will be constructed in §4.

Directly from their definition, and by the general theory of Fourier Integral Operators, we see that scFIOs have a symbol calculus. We won't write down the the details of this, since it would be largely a repetition of the corresponding results for standard FIOs. As an indication of how the theory of scFIOs reduce to that of standard FIOs, we'll simply state the following result on propagation of wave-packets and of Lagrangian scs's:

Theorem 3.3 *Let $F_k:C^\infty(M_1)\to C^\infty(M_2)$ be a scFIO associated to the admissible canonical relation Γ, and let $\{\psi_k\}$ be a Lagrangian scs associate to an admissible $\Lambda\subset T^*M_1$. Assume that Γ intersects $\Lambda\times T^*M_2$ cleanly. Then*

$$\Gamma(\Lambda)\;=\;\{\,\overline{\xi}\in T^*M_2\,;\,\exists\overline{\eta}\ \textit{such that}\ (\overline{\eta},\overline{\xi})\in\Lambda\,\}\,,$$

is an immersed Lagrangian submanifold in T^*M_2, and the sequence $\{F_k(\psi_k)\}$ is a Lagrangian scs associated to it.

By a straightforward generalization of the proof of Proposition (2.12) we obtain an oscillatory integral representation of the Schwartz kernels of a scFIO, $F=\{F_k\}$:

Lemma 3.4 *If $\phi(x,y,w)$ is a phase function locally parametrizing the Lagrangian relation associated with F, then locally the Shwartz kernel of F_k is of the form*

$$F_x(x,y)\;=\;\int e^{ik\phi(x,y,w)}\,a(x,y,w,k)\,dw\;\;+O(k^{-\infty})\,,$$

where a is a symbol as before (compactly supported in (x,y,w)). The error is in the C^∞ topology.

Observe that the estimates are microlocally on compact subsets of the Lagrangian relation associated with F. We will discuss the case of scΨDOs (the scFIOs with $M_1=M_2=M$ and Γ the diagonal) in the Appendix.

4 The Propagator.

In this section we will construct semi-classical approximations to the propagator of a Schrödinger-type operator on a manifold M. The $\hbar$-transform of the approximating operators will be an ordinary Fourier integral operator on the circle bundle $M \times S^1$. In fact the sequence of the Schwartz kernels of their Fourier coefficients will be a Lagrangian scs. The approximation will be valid in a compact range of energies, which accounts for the finite-propagation speed of singularities proper of FIOs.

The setting is as follows. Let M be a compact manifold, and consider an $\hbar$-dependent self-adjoint operator of the form

$$S_\hbar \;=\; \sum_{l=0}^{N} \hbar^l \; P_l \;, \tag{69}$$

where for each l P_l is a differential operator of order l. The symbol of $S_\hbar$ is defined to be the smooth function on T^*M

$$H(x,p) \;=\; \sum_{l=0}^{N} \sigma_{P_l}(x,p) \tag{70}$$

where σ_l is the principal symbol of P_l.

We will make henceforth the following

Assumptions:

$$\forall\,(x,p) \in T^*M \quad H(x,p) \;>\; 0\,, \quad \text{and} \tag{71}$$

$$P_N \quad \text{is elliptic.} \tag{72}$$

Remarks: (a) Condition (71) can be weakened to: H bounded below. Indeed it suffices to add a large enough constant to $S_\hbar$ to ensure (71); the reader can check that the statements of the trace formula and the propagation of semi-classical families theorem below are insensitive to the subtraction of a constant from the Hamiltonian. We assume (71) for convenience of exposition.
(b) Condition (71) does not imply that P_N must be elliptic: consider $S_\hbar = \hbar^2 D_1^2 + 1$.
(c) Condition (71) implies that the symbol of the zeroth order operator P_0 must be a positive function: $H(x,0) = \sigma_{P_0}(x) > 0$.

The ellipticity condition implies that, for every $\hbar > 0$, the spectrum of $S_\hbar$ is discrete (see below). We will denote by $\{\psi_{j,\hbar}\}$ an orthonormal basis of $L^2(M)$ of eigenfunctions of $S_\hbar$, and by $E_{j,\hbar}$ the associated eigenfunctions:

$$S_\hbar(\psi_{j,\hbar}) \;=\; E_{j,\hbar}\,\psi_{j,\hbar}\,. \tag{73}$$

The $\hbar$-transform of $S_\hbar$ is defined to be the following operator on $M \times S^1$:

$$P \;:=\; \sum_{l=0}^{N} D_\theta^{-l}\; P_l \;, \tag{74}$$

where we denote by D_θ^{-l} the obvious relative parametrix of D_θ: the operator equal to k^{-1} on the k-th eigenspace of D_θ for all non-zero k and equal to zero on the kernel of D_θ. Explicitly,

$$\left(\, D_\theta^{-1}\, u\,\right)\,(x,\theta) \;=\; \frac{i}{2\pi}\int_0^{2\pi} dt \int_0^t \;(u(x,\theta - s) - \overline{u}(x))\; ds \tag{75}$$

where

$$\overline{u}(x) \;=\; \frac{1}{2\pi}\int_0^{2\pi} \; u(x,\theta)d\theta \tag{76}$$

is the projection of u onto the kernel of D_θ. The operator D_θ^{-1} is *not* an ordinary pseudodifferential operator since D_θ is not elliptic. D_θ^{-1} is however a ΨDO with singular symbol, in the sense of Melrose-Uhlmann and Guillemin- Uhlmann, [31], [20]. It will become an ordinary ΨDO after suitable microlocalization, which amounts to the localization in energy for $S_\hbar$ alluded to above.

We call P the $\hbar$-transform of $\{S_\hbar\}$ because $\forall k \in \mathbb{Z}^+$

$$P|_{\mathcal{H}_k} \cong S_{1/k}\,, \tag{77}$$

where $\mathcal{H}_k$ is the k-th eigenspace of D_θ; indeed in $P|_{\mathcal{H}_k}$ one can replace D_θ by k, thereby obtaining $S_{1/k}$. To be more specific, let us now introduce the joint eigenvalues and eigenfunctions of the commuting pair (P, D_θ). By the previous assumptions, the operator

$$R \;=\; \sum_{l=0}^{N} D_\theta^{N-l}\, P_l \;=\; D_\theta^N P \tag{78}$$

is an N-th order *elliptic differential operator with positive symbol* equal to

$$\sigma_R\,(x,\xi;\theta,\kappa) \;=\; \sum_{l=0}^{N} \kappa^{N-l}\sigma_{P_l}(x,\xi) \;=\; \kappa^N\, H(x,\xi/\kappa)\,. \tag{79}$$

Therefore the spectrum of R is bounded below and consists of eigenvalues with finite multiplicities and converging to infinity. Let $\{\Psi_{k,j}(x,\theta)\}$ (where $k \in \mathbb{Z}$ and $j = 1, 2, \ldots$) be an orthonormal basis of $L^2(M \times S^1)$ consisting of joint eigenvectors for the pair (R, D_θ) with joint eigenvalues $\{(\lambda_{k,j}, k)\}$:

$$\begin{cases} R\Psi_{k,j} &=& \lambda_{k,j}\,\Psi_{k,j} \\ D_\theta\Psi_{k,j} &=& k\,\Psi_{k,j}\,. \end{cases} \tag{80}$$

¿From the second equation follows that $\Psi_{k,j}$ is of the form

$$\Psi_{k,j}(x,\theta) \;=\; e^{ik\theta}\,\psi_{k,j}(x) \tag{81}$$

for some function $\psi_{k,j}$ on M. Plugging back in the first equation and recalling the definition of D_θ^{-1}, get

$$R\Psi_{k,j} \;=\; e^{ik\theta}\,k^N \sum_{l=0}^{N} k^{-l}\,P_l(\psi_{k,j}) \tag{82}$$

and so the first eigenvalue equation in (80) becomes (upon division by $e^{ik\theta}k^N$)

$$S_{1/k}\,\psi_{k,j} \;=\; E_j(k)\,\psi_{k,j}\ , \quad \text{where} \quad E_j(k) \;=\; k^{-N}\,\lambda_{k,j}\,. \tag{83}$$

This procedure can be reversed, and we see that the eigenvalue problems (80) and (83) are equivalent via (81).

4.1 Energy localization

We now proceed to microlocalize P in an open cone away from $\{\kappa = 0\}$. The result is an *ordinary* ΨDO, P_f, that approximates P within a bounded range of energies. Begin by defining

$$Q \;:=\; R^{1/N}\,. \tag{84}$$

This is a first-order, elliptic, classical self-adjoint pseudodifferential operator with eigenfunctions $\Psi_{k,j}$ and eigenvalues

$$\mu_{k,j} \;=\; (\lambda_{k,j})^{1/N} \;=\; |k|\,(E_j(k))^{1/N}\,. \tag{85}$$

Lemma 4.1 *Let $f \in C_0^\infty(\mathbb{R}^+)$ be identically one on an open interval I_f and $0 \le f \le 1$ everywhere. Then the operator*

$$Q_f \;=\; f\left(D_\theta Q^{-1}\right)$$

(defined by the spectral theorem) is a classical zeroth order pseudodifferential operator whose symbol is zero in a neighborhood of $\{\kappa = 0\}$ *and*

$$\sigma_{Q_f}(x,\xi;\theta,\kappa) \;=\; f\Big(\; H(x,\xi/\kappa)^{-1/N}\Big)$$

elsewhere. Moreover:
(i) Q_f *is microlocally supported in the set*

$$\mathcal{U}_f \;=\; \{\,(x,\xi;\theta,\kappa)\;;\; H(x,\xi/\kappa)^{-1/N} \in \mathit{Supp}(f)\,\}\;, \quad \textit{and} \tag{86}$$

(ii) Q_f *is microlocally equal to the identity in the set*

$$\mathcal{V}_f \;=\; \{\,(x,\xi;\theta,\kappa)\;;\; H(x,\xi/\kappa)^{-1/N} \in I\,\}\,. \tag{87}$$

REMARKS: (a) The statement about the microlocal support of Q_f means that

$$\forall u \in \mathcal{D}'(M\times S^1) \qquad \mathrm{WF}(u)\cap\mathcal{U}_f \;=\; \emptyset \Rightarrow \mathrm{WF}\,[Q_f(u)] \;=\; \emptyset\;, \tag{88}$$

while the statement about Q_f being microlocally the identity means that

$$\forall u \in \mathcal{D}'(M\times S^1) \qquad \mathrm{WF}(u)\subset\mathcal{V}_f \Rightarrow \mathrm{WF}\,[u - Q_f(u)] \;=\; \emptyset\;. \tag{89}$$

(b) The satements (i) and (ii) in the lemma also hold for any power of Q_f.
(c) Q_f clearly commutes with both P and D_θ.

PROOF The operator inside f is a classical zeroth order self-adjoint ΨDO, and the first conclusion about Q_f is a direct application of Theorem I of the appendix of [18]. The statements (88) and (89) follow from Theorem 0.6 of [7], in the following way. The couple of operators (Q, D_θ) form a commuting elliptic pair of first-order self-adjoint pseudodifferential operators, with joint spectrum $\{(\mu_{k,j},k)\}$. Let

$$J\,: T^*(M\times S^1)\setminus\{0\} \to \mathbb{R}^2\setminus\{0\} \tag{90}$$

be the map with components $J = (q,\kappa)$ where q is the symbol of Q. The Theorem cited says the following: *Let* $u = \sum_{k,j} u_{k,j}\Psi_{k,j}$ *and* $\Gamma\subset\mathbb{R}^2\setminus\{0\}$ *be an open cone. Then*

$$\big(\forall\;(k,j)\text{ such that }(\mu_{k,j},k)\in\Gamma\;\; u_{k,j}=0\big)\;\Rightarrow\;\mathrm{WF}(u)\cap J^{-1}(\Gamma)=\emptyset\,. \tag{91}$$

Let C_f, $C_I\subset\mathbb{R}^2\setminus\{0\}$ be the cones

$$C_f \;=\; \{\,(z_1,z_2)\,;\, z_2/z_1\in\mathrm{supp}\,(f)\,\} \quad\text{and}\quad C_I \;=\; \{\,(z_1,z_2)\,;\, z_2/z_1\in I\,\}\,. \tag{92}$$

Then

$$\mathcal{U}_f \;=\; J^{-1}(C_f) \quad\text{and}\quad \mathcal{V}_f \;=\; J^{-1}(C_I)\,, \tag{93}$$

and $\forall\;(k,j)$

$$(\mu_{k,j},k)\notin C_f \Rightarrow Q(\Psi_{k,j}) \;=\; 0\,,\quad\text{while}\quad (\mu_{k,j},k)\in C_I \Rightarrow Q(\Psi_{k,j}) \;=\; \Psi_{k,j}\,. \tag{94}$$

Consider now $u\in\mathcal{D}'(M\times S^1)$, write $u = \sum_{k,j} u_{k,j}\Psi_{k,j}$ and $Q(u) = \sum_{k,j} a_{k,j}\Psi_{k,j}$. By (94), $\forall(k,j)$

$$(\mu_{k,j},k)\notin C_f \Rightarrow a_{k,j} \;=\; 0\,,\quad\text{and}\quad (\mu_{k,j},k)\in C_I \Rightarrow a_{k,j} \;=\; u_{k,j}\,. \tag{95}$$

(88) and (89) follow easily from statements (91) through (95).

□

We will use the operator Q_f to microlocalize the operator P. As mentioned earlier, the operator D_θ^{-1} is a pseudodifferential operator with singular symbol. Precisely, its Schwartz kernel is in a class $I^{p,l}((M\times S^1)^2,\Lambda_0,\Lambda_1)$ of singular Lagrangian distributions of Guillemin and Uhlmann, where Λ_0 is the conormal to the diagonal in $(M\times S^1)^2$ and Λ_1 if the flow-out from $\{\kappa = 0\}$. We refer the reader to [20] for the theory of such distributions. The properties of these operators that we presently need are: (1) they are stable under the action of FIOs, and in particular ΨDOs, and (2) microlocally away form the intersection $\Lambda_0\cap\Lambda_1$ they are ordinary Fourier integral operators. These facts together with Lemma 4.1 imply:

Lemma 4.2 *The operator*

$$B \;:=\; Q_f\, D_\theta^{-1} \tag{96}$$

is a classical pseudodifferential operator of order (-1)*. Moreover* B *is microlocally supported in* $\mathcal{U}_f$ *and it is microlocally equal to* D_θ^{-1} *in* $\mathcal{V}_f$*.*

We now define the microlocalized version of P:

$$P_f \;:=\; B^N\, R \;=\; B^N \sum_{l=0}^{N} D_\theta^{N-l}\, P_l \ , \tag{97}$$

which is easily seen to equal

$$P_f \;=\; Q_f^N\, P\, . \tag{98}$$

The Fourier coefficients of P_f are (with $\hbar = 1/m$)

$$\Big(P_f\Big)_m \;=\; [\, f(S_\hbar)^{-1/N}\,]^N\, S_\hbar\, . \tag{99}$$

We summarize the properties of P_f that we need in the following:

Proposition 4.3 *The operator* P_f *is a classical zeroth order pseudodifferential operator on* $M \times S^1$ *commuting with* D_θ*. It is microlocally supported in* $\mathcal{U}_f$ *and it is microlocally equal to* P *in* $\mathcal{V}_f$*. In particular, in* $\mathcal{V}_f$ *its symbol is*

$$\sigma_{P_f}|_{\mathcal{V}_f}(x,\xi;\theta,\kappa) \;=\; H(x,\xi/\kappa)\ . \tag{100}$$

In the next paragraph we use P_f to approximate $\exp itD_\theta P$.

4.2 Propagation of sc states

As a first application of the previous construction of P_f, we will now prove the following theorem:

Theorem 4.4 *Let* $\Lambda_0 \subset T^*M$ *be an admissible Lagrangian (resp. isotropic) submanifold, and let* $\{\psi_m\}$ *be an associated Lagrangian (resp. Hermitian) semi-classical state. Then, for every* t*, the family*

$$\{\, \exp(-itmS_{1/m})(\psi_m)\, \} \tag{101}$$

is a Lagrangian (resp. isotropic) family associated to the manifold $\phi_t(\Lambda_0)$*, where* $\{\phi_t\}$ *denotes the Hamilton flow of* $H(x,p)$*.*

Remarks: (1) The exponential appearing in (101) is the fundamental solution of Schrödinger's equation

$$i\hbar\frac{\partial u}{\partial t} \;=\; S_\hbar\,(u)$$

with $\hbar = 1/m$. Again, the restriction of $\hbar$ to the reciprocals of integers is inessential.

(2) Although we won't do so here, we could compute the symbol of the image family. For the wave packets of §2 this yields formulae analogous to those of Cordoba-Fefferman and Hagedorn, [9], [22]. See [33] for estimates of matrix elements between a wave packet and the eigenfunctions of the Hamiltonian.

The proof of this Theorem is based on the following lemma:

Lemma 4.5 *Let* $f \in C_0^\infty(\mathbb{R}^+)$ *and let* $\psi \in \mathcal{D}'(M \times S^1)$ *be such that* $WF(\psi) \subset \mathcal{V}_f$*. Then*

$$[\; e^{itD_\theta P} - e^{itD_\theta P_f}\;]\;(\psi)$$

is smooth.

PROOF Write $e^{itD_\theta P_f} - e^{itD_\theta P} = e^{itD_\theta P}\left[e^{itT} - I\right]$, where $T = D_\theta(P_f - P) = D_\theta P(Q_f^{2N} - I)$. Then $\Psi := \left[e^{itT} - I\right](\psi)$ can be written as

$$\Psi = ie^{itT}\left(\int_0^t e^{-isT}\, T(\psi)\, ds\right)$$

(Duhamel's principle). Since $\mathrm{WF}(\psi) \subset \mathcal{V}_f$, $Q_f^{2N}\psi - \psi$ is smooth; hence $T(\psi)$ is smooth. Since the operator $\exp(isT)$ maps smooth functions into smooth functions, Ψ is smooth and hence

$$\left[\, e^{itD_\theta P} - e^{itD_\theta P_f} \,\right](\psi) = -e^{itD_\theta P}(\Psi)$$

is smooth.

□

Although we won't need it right away, we note the following corollary that we will use in the proof of the trace formula:

Corollary 4.6 *With the notations of Lemma 4.1, let $f, g \in C_0^\infty(\mathbb{R}^+)$ be such that $supp(f) \subset I_g$. Then*

$$\left[\, e^{itD_\theta P} - e^{itD_\theta P_g} \,\right] Q_f \tag{102}$$

is a smoothing operator.

PROOF OF THEOREM 4.4 Choose $f \in C_0^\infty(\mathbb{R})$ as in §3.1, making sure that the set $\mathcal{V}_f$ contains Λ, the horizontal lift of Λ_0 with respect to which the $\hbar$-transform of $\{\psi_m\}$ is Lagrangian (resp. Hermitian). This is indeed possible since by admissibility Λ is a closed conic set in Σ. From the lemma follows that the $\hbar$ transform of $\{\, \exp(itmS_{1/m})(\psi_m)\,\}$ and

$$\exp(itD_\theta P_f)\,(\psi)\ , \tag{103}$$

where ψ is the $\hbar$ transform of $\{\psi_m\}$, differ by a smooth function on $M \times S^1$, and hence one is a Lagrangian (resp. Hermitian) sc state iff the other one is. We have seen that Q_f is a classical self-adjoint zeroth order pseudodifferential operator, so $W = D_\theta P_f$ is a first order operator and $\exp(itW)$ is a Fourier integral operator whose canonical relation is the graph of G_t, the time t map of the Hamilton flow of the symbol of W. By the invariance of Lagrangian (resp. Hermitian) distributions under FIO's associated to canonical graphs, we conclude that the $\hbar$ transform of (101) is a Lagrangian (resp. Hermitian) distribution associated to $G_t(\Lambda)$. On $\mathcal{V}_f$ however the symbol of W is

$$\kappa\, H(x, \xi/\kappa)\ ,$$

from which it is clear that the reduction of $G_t(\Lambda)$ is $\phi_t(\Lambda_0)$, and the proof of the Theorem is complete.

□

The sequence of Fourier coefficients of the Schwartz kernel of the operator $\exp(itD_\theta P_f)$ is therefore a Lagrangian semi-classical family associated to the graph of the flow at time t of the reduction of the symbol of P_f. The latter agrees with the classical Hamiltonian an the open set of the form $H^{-1}(E_1, E_2)$, and is zero outside a larger set of the same form.

We finish with a local oscillatory integral representation of the Shwartz kernel of the operator $\mathcal{U}_f := \exp(itD_\theta P_f)$. We are only interested in an expression valid microlocally in the open cone $\mathcal{V}_f$, which is invariant under the Hamilton flow of the symbol of $D_\theta P_f$. By the previous paragraph and Lemma (3.4), microlocally in the open set

$$X_I := \{\, (x,p) \in T^*M\ ;\ H(x,p)^{-1/N} \in \mathrm{int} I\,\}$$

(which is invariant under the Hamilton flow of H) the Schwartz kernel of the operators $\mathcal{U}_{f,m} = \exp(itm(P_f)_m)$ can be written as oscillatory integrals of the form

$$\int e^{im\psi(t,x,y,w)}\, a(t,x,y,w;m)\, dw$$

where ψ is a non-degenerate phase function parametrizing the graph of the Hamilton flow of H in X_I. For $|t|$ small, it is natural to take ψ of the form

$$\psi(t,x,y,w) \;=\; S(t,x,w) - y\cdot w$$

where S is the solution of the Hamilton-Jacobi equation

$$\begin{cases} \frac{\partial S}{\partial t} + H(x,\nabla_x S) & = \quad 0 \\ S(t=0,x,w) & = \quad x\cdot w \end{cases}$$

The resulting expression (valid for small time) is well known on $\mathbb{R}^n$, in the theory of Helffer and Robert, [24]. (See also recent work of Meinrenken, [30], for an extension of that theory to all t). Our formulation however shows that $\mathcal{U}_f$ is globally a Lagrangian distribution, and therefore can be treated with standard FIO techniques.

5 The Semiclassical Trace Formula

5.1 The statement

The setting and notations in this section are the same as is §3: we consider a Schrödinger-type operator $S_\hbar$ on a compact manifold M with associated classical Hamiltonian $H(x,p)$ a smooth function on T^*M. Both assumptions (71) and (72) will be in effect.

The semiclassical trace formula (STF) is a statement about the asymptotic distribution of the spectral data of $S_\hbar$, as $\hbar \to 0$, more precisely, about the asymptotic behavior of sums of the form

$$\sum_{j=1}^{\infty} < A_\hbar\, \psi_{j,\hbar}, \psi_{j,\hbar} > \varphi\left(\frac{E_{j,\hbar}-E}{\hbar}\right) \qquad \text{as } \hbar \to 0\,. \tag{104}$$

This formula generalizes results of Chazarin, [4], Colin de Verdière, [5], and Duistermaat-Guillemin, [15], in the context of large-eigenvalue asymptotics of an elliptic operator. Recent work on the STF on $\mathbb{R}^n$, using different techniques, has been done by Meinrenken, [30] and Dozias, [11].

In (104) $A_\hbar$ is an $\hbar$-admissible zeroth order pseudodifferential operator (c.f. appendix), φ is a test function and E is a parameter. Each periodic trajectory with action $\oint_\gamma pdq$ in the support of $\hat{\varphi}$ contributes to the small $\hbar$ behavior of (104). In the proof, we analyze the contribution of the trajectories with a given action, and then sum the estimates. Accordingly, we will assume that the Fourier transform of φ, $\hat{\varphi}$, is in $C_0^\infty(\mathbb{R})$. This restriction on φ is the main difference between our result and Gutzwiller's trace formula, [21]. The restriction is necessary, in the sense that the sum of the contributions of infinitely-many trajectories in general is divergent.

The remaining assumptions in the STF are on the Hamilton flow of H on the energy shell

$$\Sigma_E := H^{-1}(E)\,. \tag{105}$$

To begin with, we assume:

$$E \;\text{ is a regular value of } H\,, \tag{106}$$

so that Σ_E is a smooth $(2n-1)$-dimensional manifold. It is compact by the ellipticity assumption and the compactness of M. Physically, this assumption says that there are no equilibria with energy E. Without this assumption, the asymptotics of (104) can include logarithmic terms in $\hbar$, and half-integral powers of $1/\hbar$; with R. Brummelhuis we have analyzed a first case of this situation in [3]. Finally, we'll assume

$$\text{the Hamilton flow of } H \text{ is clean on } \Sigma_E\,, \tag{107}$$

a notion that we now recall.

Definition 5.1 *The Hamilton flow of H, $\{\phi_t\}$, is said to be clean on Σ_E iff:*

1. *The set*

(108) $$\mathcal{P} \;:=\; \{\,(z,T)\in\Sigma_E\times\mathbb{R}\,;\,\phi_T(x)=x\,\}$$

is a submanifold of $\Sigma_E\times\mathbb{R}$ *(the dimension is allowed vary from one connected component to another), and*

2. *For every* $(z,t)\in\mathcal{P}$ *the tangent space* $T_{(z,T)}\mathcal{P}$ *is the set of all* $(\zeta,\tau)\in(T_z\Sigma_E)\times\mathbb{R}$ *such that*

(109) $$\tau\Xi_z + d(\phi_T)_z(\zeta) \;=\; \zeta\,.$$

Remarks: (a) The dimensions of the various connected components of $\mathcal{P}$ can range from one, dimension of a component of the form $\gamma\times\{T\}$ where γ is an isolated trajectory, to $(n-1)$, corresponding to the component $\Sigma_E\times\{0\}$. (b) Condition 2 in the previous definition, applied to a connected component of $\mathcal{P}$ of the form $\gamma\times\{T\}$, is equivalent to the non-degeneracy of γ. (c) Equation (109) is the differentiated version of equation $\phi_T(z)=z$.

In order to state the STF, we need to review two facts implied by the "cleanness" assumption.

Lemma 5.2
1. *With the notation* $\phi_t(z)=(q(t),p(t))\in T^*M$*, the map*

(110) $$\begin{array}{rcl}\mathcal{P} & \to & \mathbb{R}\\ (z,T) & \mapsto & \int_0^T p\dot{q}\,dt\end{array}$$

is locally constant, (i.e. it's constant on each connected component of $\mathcal{P}$*).*
2. *The connected components of* $\mathcal{P}$ *inherit smooth densities.*

Part 1 is classical: all members of a smooth family of periodic trajectories have the same action. For part 2 in general we refer to [19], Lemma 2.7; here we will simply describe the densities in the following three cases:

1. For the connected component $\Sigma_E\times\{0\}$, the density is the Liouville density on Σ_E.
2. For the connected component $\gamma\times\{T\}$ corresponding to a non-degenerate trajectory, the density is

   (111) $$\frac{dt}{\sqrt{|\det(I-P_\gamma)|}}$$

   where t is the time variable along the trajectory (with an arbitrary initial condition) and P_γ is the linearized Poincaré map of γ.
3. In case the Hamilton flow of H on Σ_E is periodic, let $T^{\#}:\Sigma_E\to\mathbb{R}$ be the "primitive period" function. Then the connected components of $\mathcal{P}$ are of the graphs of the maps mT_0, $m\in\mathbb{Z}$, and as such are naturally identified with Σ_E itself. Under that identification, the density is just the Liouville density on Σ_E (see [38], section 3.4.1).

Finally, the formula involves the sub-principal symbol of $S_\hbar$, which is

(112) $$H_{\text{sub}}(x,p) \;=\; \sum_{l=0}^{N}\sigma_{s,l}\,(x,p)$$

where $\sigma_{s,l}$ is the subprincipal symbol of P_l. From H_{sub} we define a function, β, on $\mathcal{P}$, by averaging it:

(113) $$\begin{array}{rcl}\beta:\mathcal{P} & \to & \mathbb{R}\\ (z,T) & \mapsto & \int_0^T H_{\text{sub}}\pi_t(z)\,dt\,.\end{array}$$

We are now ready to state the STF:

Theorem 5.3 *Under the assumptions (106) and (107), for each test function φ such that $\hat{\varphi} \in C_0^\infty(\mathbb{R})$ and each $\hbar$-admissible zeroth-order pseudodifferential operator $A_\hbar$, the sum (104) has an asymptotic expansion as $\hbar \to 0$ of the form*

$$\sum_{j=1}^{\infty} < A_\hbar \psi_{j,\hbar}, \psi_{j,\hbar} > \varphi\left(\frac{E_{j,\hbar} - E}{\hbar}\right) \sim \sum_\nu e^{i\alpha_\nu \hbar^{-1}} \hbar^{-d_\nu} e^{\pi i m_\nu/4} \sum_{j=0}^{\infty} c_{\nu,j} \hbar^j , \tag{114}$$

where:

1. *The sum $\sum_\nu$ is over the connected components, $\mathcal{P}_\nu$, of $\mathcal{P}$ containing at least a point (z, T) with T in the support of $\hat{\varphi}$. This sum is finite.*
2. *$d_\nu = (dim\, \mathcal{P}_\nu - 1)/2$.*
3. *m_ν is an integer, the common Maslov index of the trajectories in $\mathcal{P}_\nu$, and finally*
4. *The leading coefficient of the ν-th term is*

$$c_{\nu,0} \;=\; (2\pi)^{-(d\nu+1)/2} \int_{\mathcal{P}_\nu} e^{i\beta}\, a\, \hat{\varphi}(T)\, d\mu_\nu\,. \tag{115}$$

where $d\mu_\nu$ is the natural density on $\mathcal{P}_\nu$ and a the principal symbol of $A_\hbar$.

Remarks. (a) In the integral (115), the function $\hat{\varphi}$ is considered as a function of the second variable, T, on $\mathcal{P}_\nu \subset \Sigma_E \times \mathbb{R}$, while a and β are functions of the first. In each of the cases above, the result of the integral is as follows:

1. For the component $\Sigma_E \times \{0\}$, the integral is $\hat{\varphi}(0) \int_{\Sigma_E} a d\lambda$, where $d\lambda$ is the Liouville measure of Σ_E.
2. For the component $\gamma \times \{T\}$ where γ is non-degenerate, the integral equals

$$\hat{\varphi}(T) \frac{1}{\sqrt{|\det(I - P_\gamma)|}} \int_0^{T^\#} e^{i\beta}\, a(q(t), p(t)) dt\,, \tag{116}$$

where $T^\#$ is the primitive period of γ.

3. In case the flow on Σ_E is periodic with primitive period function $T^\#$, the integral over the m-th component is

$$\int_{\Sigma_E} e^{i\beta}\, a(z)\, \hat{\varphi}\left(mT^\#(z)\right)\, d\lambda_z\,. \tag{117}$$

(b) The degree d_ν is zero for a non-degenerate periodic trajectory, and $(n-1)$ for $\Sigma_E \times \{0\}$.

Applying the technique of [2] of passing to a compact manifold, one immediately gets:

Corollary 5.4 *For a Schrödinger operator $-\hbar^2\Delta + V$ on $\mathbb{R}^n$ with $V \in C^\infty$ bounded below, if $E < \limsup_{|x|\to\infty} V(x)$, the above statements remain true of the sums*

$$\sum_{j;|E_{j,\hbar} - E| \leq \hbar^{1-\epsilon}} \varphi\left(\frac{E_{j,\hbar} - E}{\hbar}\right)$$

for any $0 < \epsilon < 1$.

5.2 The $\hbar$ transform of the spectral function

In the setting of the last section, let us introduce the notation

$$E_j(k) := E_{j,1/k} \quad \text{and} \quad A_j(k) := < A_{1/k}\,\psi_{j,1/k}, \psi_{j,1/k} > . \tag{118}$$

In accordance with the spirit of this paper and [19], we will study the asymptotic behavior of

$$\sum_{j=1}^{\infty} A_j(k)\,\varphi(k(E_j(k)-E)) \qquad \text{as } k \to \infty \tag{119}$$

by studying the singularities of the Fourier series with coefficients (119), namely

$$\Upsilon_E(s) = \sum_{k=0}^{\infty}\sum_{j=1}^{\infty} A_j(k)\,\varphi(k(E_j(k)-E))\,e^{iks} . \tag{120}$$

We call this distribution *the $\hbar$ transform of the spectral function.* Our immediate goal is to show how, up to a smooth function, Υ_E can be constructed from the Schwartz kernel of the approximation to the propagator of §3.3.

We first must say a few words about the matrix coefficients $A_j(k)$. By the definition of $\hbar$-admissible ΨDO of the Appendix, there exists a zeroth order, classical ΨDO on $\mathcal{M}$, A, which commutes with D_θ and such that for every $k \in \mathbb{Z}^+$ the operator $A_{1/k}$ is the restriction of A to $L^2(M) \otimes (\mathbb{C}\,e^{ik\theta})$.

Proposition 5.5 *Let $\mathcal{M} = M \times S^1$, and define the operator*

$$\mathcal{F}_E : C^\infty(S^1 \times \mathbb{R} \times \mathcal{M} \times \mathcal{M}) \to C^\infty(S^1)$$

by the formula

$$\mathcal{F}_E(u)(s) = \int u(s-tE, t, z, z)\,\hat{\varphi}(t)\,dt\,dz \tag{121}$$

where $z = (x,\theta)$ denotes the variable in $\mathcal{M}$. Choose $f, g \in C_0^\infty(\mathbb{R}^+)$ as in Corollary 4.6 and such that $E^{-1/N} \in I_f$, and let $\mathcal{K}_{f,g}(s,t,z,z')$ denote the Schwartz kernel of $A\,Q_f\,e^{iD_\theta(tP_g+sI)}$. Then $\mathcal{F}_E$ extends by continuity to a class of distributions containing $\mathcal{K}_{f,g}$ and

$$\Upsilon_E = \mathcal{F}_E(\mathcal{K}_{f,g}) \qquad \textit{modulo } C^\infty(S^1) . \tag{122}$$

We will break the proof into a series of lemmas. If $\chi \in C_0^\infty(\mathbb{R}^+)$, define

$$\Upsilon_E^\chi(s) = \sum_{k=1}^{\infty}\sum_j A_j(k)\,\chi(E_j(k))\,\varphi(k(E_j(k)-E))\,e^{iks} . \tag{123}$$

Lemma 5.6 *If $\chi \in C_0^\infty(\mathbb{R})$ is identically 1 on an interval I containing E in its interior and $0 \le \chi \le 1$ elsewhere, then*

$$\sum_j A_j(k)\,\chi(E_j(k))\,\varphi(k(E_j(k)-E)) - \sum_j A_j(k)\,\varphi(k(E_j(k)-E)) = O(k^{-\infty}) , \tag{124}$$

where the estimate is locally uniform in E. Hence $\Upsilon_E - \Upsilon_E^\chi$ is a smooth function.

PROOF To lighten-up the notation a bit, we'll take $A_j(k) = 1$; all we need for the proof is that the matrix coefficients are bounded by a constant independent of j and k, because A is zeroth order.

We must show the rapid decrease in k of

$$\sum_j (1-\chi)(E_j(k))\,\varphi(k(E_j(k)-E)) = \sum_{j;\,E_j \notin I} (1-\chi)(E_j(k))\,\varphi(k(E_j(k)-E)) . \tag{125}$$

We will first establish the rough estimate

$$\exists\, C,\, l,\, m \quad \forall\, \lambda,\, k \qquad \#\{\, j\,;\, \lambda \leq E_j(k) \leq \lambda + 1\,\} \leq C\, \lambda^l\, k^m\,, \tag{126}$$

which is a consequence of standard Weyl-type estimates on the eigenvalues of the elliptic differential operator R (defined in (78)). More specifically, recall that the eigenvalues of R are the numbers $k^N E_j(1/k)$, indexed by pairs of indices (k, j). There exists then a constant C such that $\forall \lambda'$

$$\#\{\, (j,k)\,;\, \lambda' \leq k^N E_j(k) \leq \lambda' + 1\,\} \leq C\, (\lambda' + 1)^{(n/N)} \tag{127}$$

(see for example [36] Theorem 21.2). Fix now k and set $\lambda' = k^N \lambda$. Since the pairs (j,k) in the set (127) with a given k are not more than with k variable, get the inequality

$$\#\{\, j\,;\, \lambda \leq E_j(k) \leq \lambda + 1/k^N\,\} \leq C\, (k^N \lambda + 1)^{(n/N)}\,. \tag{128}$$

Summing k^N of such estimates, each for the number of $E_j(k)$ ranging in an interval of length k^{-N} between λ and $\lambda + 1$, gives

$$\#\{\, j\,;\, \lambda \leq E_j(k) \leq \lambda + 1/k^N\,\} \leq C\, k^N\, \left(\, k^N(\lambda + 1) + 1\right)^{(n/N)} \tag{129}$$

with the same constant and for all λ, k. This proves (126). Now recall that φ is rapidly decreasing. Let $\epsilon > 0$ be such that $[E - \epsilon, E + \epsilon] \subset I$. Since

$$\forall\, p > 0 \;\; \exists\, C_p > 0 \;\; \forall\, t \notin [-\epsilon, \epsilon] \qquad |\varphi(t)| \leq C_p\, |t|^{-p}\,, \tag{130}$$

then $\forall p > 0$ and $\forall E_j \notin I$

$$|\varphi(k(E_j(k) - E))| \leq C_p\, k^{-p}\, |E_j(k) - E|^{-p}\,. \tag{131}$$

It follows that the absolute value of (125) is less than or equal to

$$\sum_{j;E_j \notin [E-\epsilon, E+\epsilon]} |\, \varphi\, (k(E_j(k) - E))\,| \leq C_p\, k^{-p}\, (I + II)\,, \tag{132}$$

where

$$I \;=\; \sum_{0<E_j<E-\epsilon} |E_j(k) - E|^{-p} \quad \text{and} \quad II \;=\; \sum_{E_j>E+\epsilon} |E_j(k) - E|^{-p}\,. \tag{133}$$

We now use the rough bound (126) to estimate these sums. First $\exists C_1$ such that

$$I \leq \#\{\, j\,;\, E_j(k) \leq E - \epsilon\,\}\, (E - \epsilon)^{-p} \leq C_1\, k^m\, (E - \epsilon)^{-p}. \tag{134}$$

Secondly,

$$\begin{aligned} II \;&\leq\; \textstyle\sum_{r=0}^{\infty} \sum_{\epsilon+r+1>E_j-E\geq\epsilon+r} (E_j(k) - E)^{-p} \\ &\leq\; Ck^m \textstyle\sum_{r=0}^{\infty} (\epsilon + r)^{l-p}\,. \end{aligned} \tag{135}$$

Hence if we define

$$\tilde{C_p} \;=\; C_p \left(C_1\, (E - \epsilon)^{-p} + C \sum_{r=0}^{\infty} (\epsilon + r)^{l-p} \right)$$

(which is finite if $p \geq l + 2$) we have

$$\sum_{j;E_j \notin [E-\epsilon, E+\epsilon]} |\, \varphi\, (k(E_j(k) - E))\,| \leq \tilde{C_p}\, k^{m-p}\,.$$

Since we can choose p arbitrarily large, we have established the rapid decrease of (125); local uniformity on E is obvious from the proof.

□

We now pick $\chi^f(x) = f(1/x^N)$ where $f \in C_0^\infty(\mathbb{R}^+)$. We record the following consequence of the definitions (recall that Q_f commutes with P and D_θ):

Lemma 5.7 *With the previous choice of* χ

$$\Upsilon_E^{\chi^f}(s) = \sum_{k=0}^{\infty}\sum_j < A\, Q_f \Psi_{k,j}, \Psi_{k,j} > \varphi(k(E_j(k) - E))\, e^{iks}\,. \tag{136}$$

Turning to the operator $\mathcal{F}_E$:

Lemma 5.8 $\mathcal{F}_E$ *is a Fourier integral operator associated with the canonical relation* $\mathcal{C}_E \subset T^*S^1 \times T^*(S^1 \times \mathbb{R} \times \mathcal{M} \times \mathcal{M})$ *set of all points of the form*

$$(\,(s = \theta + tE, \kappa)\ ,\ (\theta, \kappa\,;\, t, \kappa E\,;\, \overline{x}\,;\, \overline{x})\,)$$

with $\overline{x} \in T^*\mathcal{M}$ *and* $t \in \operatorname{supp} \hat{\varphi}$*. In particular,* $\mathcal{F}_E$ *extends by continuity to distributions* $u \in \mathcal{D}'(\mathcal{M})$ *satisfying*

$$WF(u) \cap \{\,\kappa = 0\,\} \;=\; \emptyset. \tag{137}$$

Proof The Schwartz kernel of $\mathcal{F}$ is locally given by oscillatory integrals of the form

$$\hat{\varphi}(t) \int e^{i\,[\kappa(s - tE) \,+\, (x - y)\cdot\xi]}\; d\xi d\kappa. \tag{138}$$

□

Next we construct the right-hand side of (136) from the Schwartz kernel of the operator $A\, Q_f\, e^{iD_\theta(tP + sI)}$.

Lemma 5.9 $\Upsilon_E^{\chi^f}$ *is the result of applying* $\mathcal{F}_E$ *to the Schwartz kernel of the operator* $A\, Q_f\, e^{iD_\theta(tP+sI)}$.

Proof Notice that since the microlocal support of Q_f does not intersect the set $\{\kappa = 0\}$, one can indeed apply the operator $\mathcal{F}_E$ to the Schwartz kernel of $Q_f\, e^{iD_\theta(tP+sI)}$. The latter is

$$\sum_k \sum_j e^{ik(tE_j(k)+s)} (A \circ Q_f)(\Psi_{k,j})(z)\, \overline{\Psi_{k,j}(z')}\,,$$

and an easy calculation shows that applying $\mathcal{F}_E$ to this series term by term yields $\Upsilon_E^{\chi^f}$.

□

Proof of Proposition 5.5. By Corollary 4.6,

$$\mathcal{F}_E\, \left(A\, Q_f\, e^{isD_\theta} \left[e^{itD_\theta P} - e^{itD_\theta P_g}\right]\right) \in C^\infty(S^1)\,. \tag{139}$$

By lemmas 5.6 and 5.9, the proof of Proposition 5.5 is complete.

5.3 Proof of the trace formula

Proposition 5.5 reduces the problem of studying the singularities of Υ_E to a problem of composing two Fourier integral operators: we must show that, under the hypotheses of the trace formula, the result of applying $\mathcal{F}_E$ to $\mathcal{K}_{f,g}$ is a Lagrangian distribution. We must then locate its singularities, and compute the associated symbols. Finally, one uses an elementary fact that the Fourier coefficients of a Lagrangian distribution on the circle have an asymptotic expansion governed by the singularities of the distribution. All this analysis is in fact identical to that contained in [19], here we will simply highlight the main features for completeness. We will continue to use the notation $\mathcal{M} = M \times S^1$.

Theorem 5.10 *Without having to assume (106) or (107), the distribution* $\mathcal{K}_{f,g}$ *is a Lagrangian distribution on* $S^1 \times \mathbb{R} \times \mathcal{M} \times \mathcal{M}$*, with associated Lagrangian submanifold,* Γ*, set of all points* $(s, \sigma\,;\, t, \tau\,;\, \overline{x}\,:\, \overline{y}) \in \dot{T}^*S^1 \times \dot{T}^*\mathbb{R} \times \mathcal{U}_f \times \mathcal{U}_f$ *such that, with the notation* $\overline{x} = (x, \xi; \theta, \kappa)$ *and* $\overline{y} = (y, \eta; \theta, \kappa')$

$$\begin{array}{rcl} s & = & \theta + tE \\ \overline{y}' & = & \phi_t(\overline{x}) \end{array} \tag{140}$$

Corollary 5.11 *Without having to assume (106) or (107), the wave-front set of* Υ *is contained in the set of all* (s,σ) *such that* $\kappa > 0$ *and* $\exists z \in \Sigma_E$, $T \in supp\,\hat{\varphi}$ *such that*

$$\phi_t(z) = z \quad \textit{and} \quad s = \int_0^T p\,\dot{q}\,dt$$

where $\phi_t(z) = (q(t), p(t))$.

By the composition Theorem of Fourier integral operators, $\mathcal{F}_E(\mathcal{K}_{f,g})$ is a Lagrangian distribution provided $\mathcal{C}_E$ meets Γ cleanly, see [19] for the precise meaning of this. Because of the simple θ dependence in all the operators, this condition reduces to one in T^*M:

Proposition 5.12 *The clean intersection condition [25] ensuring that the result of applying* $\mathcal{F}_E$ *to* $\mathcal{K}_{f,g}$ *is a Lagrangian distribution is equivalent to (106) and (107).*

Proceeding exactly as in [19] (the only difference being the presence of the ΨDO A, which at the symbolic level merely multiplies the symbol of $\exp(iD_\theta(tP_g + s\mathrm{Id})$ by a) one proves the Theorem with $\hbar \to 0$ along the values $\hbar = 1/k$. It remains to show that the estimates are valid as $\hbar \to 0$ continuously.

For that effect consider, for $\alpha \in (0,1)$,

$$\Upsilon_\alpha(s) = \sum_{k=0}^{\infty}\sum_j < A\,Q_f\Psi_{k,j}, \Psi_{k,j} > \varphi\Big((k+\alpha)\,(E_j(1/(k+\alpha)) - E)\Big)\, e^{i(k+\alpha)s}\,. \tag{141}$$

This is the Υ of [19] associated to the pair of commuting operators $D_\theta + \alpha$ and $D_\theta P_f$. Observe that the dependence on α is at the subprincipal symbol level. Therefore the dependence on α in the oscillatory integral representation of Υ_α is only on the amplitude (not the phase), and the amplitude clearly depends smoothly on α. Therefore the estimates on the Fourier coefficients of $\Upsilon_\alpha(s)e^{-i\alpha s}$ are uniform in α, which amounts to the desired estimates as $\hbar \to 0$ continuously in the trace formula. This argument is a direct analogue of Colin de Verdière's in [7], Theorem 4.4.

6 Variations on the STF

We have gathered below three variations on the STF. The last two are generalizations of Theorem 2.3 in [2] and Theorem 6.3 in [37], respectively, to the present setting; the main difference is that the present results contain no square roots of the eigenvalues, which have no sense physically. The proofs of these generalizations are identical to those of the original Theorems, one simply has to work with the approximant $AQ_f\exp[itD_\theta(tP_g + sI)]$ of §4. Therefore we simply state the results.

6.1 The STF and the Bohr-Sommerfeld condition.

We place ourselves in the setting of the STF. Then Υ is a distribution on the circle with finitely-many classical conormal singularities at the points $exp(it\oint_\gamma pdq)$, where γ is a periodic trajectory on Σ_E with period in the support of $\hat{\varphi}$. Hence the singularity of Υ created by γ is at $1 \in S^1$ iff γ satisfies the Einstein-Bohr-Sommerfeld quantization condition that

$$\oint_\gamma pdq \in 2\pi\mathbb{Z}\,. \tag{142}$$

In this section we exploit this fact to prove that the *averages* of the Fourier coefficients of Υ have a leading asymptotic behavior governed by the periodic trajectories satisfying (142). The idea is to apply Féjer summation to the Fourier series of Υ:

Lemma 6.1 *Suppose the numerical sequence (a_k) has the asymptotic behavior*

$$a_k \sim c_0\,\omega^k\,k^d + O(k^{d-1}) \qquad \text{as } k \to \infty\,. \tag{143}$$

where $\omega \in S^1$ is a complex number of modulus one. Then, if $\omega \neq 1$

$$\frac{1}{m}\sum_{k=1}^{m} a_k \sim \begin{cases} c_0\,m^{d-1}\,\frac{\omega^{m+1}}{\omega-1} + O(k^{d-1}) & \text{if } d > 0 \\ c_0\,m^{d-1}\,\frac{\omega^{m+1}}{\omega-1} + O(k^{-1}\log k) & \text{if } d = 0\,, \end{cases} \tag{144}$$

while if $\omega = 1$,

$$\frac{1}{m}\sum_{k=1}^{m} a_k \sim \frac{c_0}{d+1}\,m^d + O(m^{d-1})\,. \tag{145}$$

PROOF If $b_k = O(k^{d-1})$, then $\frac{1}{m}\sum_{k=1}^m b_k$ is $O(m^d - 1)$ if $d > 0$ and $O(m^{-1}\log m)$ if $d = 0$, so WLOG $a_k = c_0\,\omega^k\,k^d$. But then, if $\omega \neq 1$,

$$\frac{1}{m}\sum_{k=1}^{m} a_k = c_0\left(\omega\frac{\partial}{\partial\omega}\right)^d \frac{\omega^{m+1}-1}{\omega-1}\,. \tag{146}$$

(Here of course we are abusing the notation, regarding ω as a variable, what we mean is an identity of functions evaluated at the comlex number ω.) The estimates (144) follow easily.

□

As corollary we obtain:

Corollary 6.2 *Besides the assumptions of the STF assume $\hat\varphi \in C_0^\infty(\mathbb{R})$ vanishes to order $n = dim(M)$ at zero. Let*

$$L(\varphi, m) := \frac{1}{m}\sum_{k=1}^{m}\sum_j \varphi\left(k(E_j(k) - E)\right)\,. \tag{147}$$

Then:
(a) If there is no periodic trajectory $\gamma \subset \Sigma_E$ whose action is in $\pi\mathbb{Q}$ and satisfying $\hat\varphi(T_\gamma) \neq 0$, then

$$L(\varphi, m) = O(1/m)\,. \tag{148}$$

(b) Suppose $\mathcal{P}_\nu \subset \mathcal{P}$ is connected component of action $S \in 2\pi\mathbb{Z}$, and that all other such components have dimension strictly less than dim $\mathcal{P}_\nu$. Then

$$L(\varphi, m) = m_\nu^d\,\frac{c_{\nu,0}}{d_\nu + 1} + R(m)\,, \tag{149}$$

where $c_{\nu,0}$ is the coefficient (115) (with $a = 1$), $d_\nu = (dim\mathcal{P}_\nu - 1)/2$ and

$$R(m) = \begin{cases} O(m^{d_\nu - 1}) & \text{if } d_\nu \geq 1 \\ O(\log(m)/m) & \text{if } d_\nu = 0 \end{cases} \tag{150}$$

The proof follows from the STF and the previous lemma.

6.2 Estimates Uniform in E.

In Theorem 5.3, the parameter E was constant: Assumptions on $H^{-1}(E)$ translate into estimates with fixed E. Here we show that assumptions on a band of energies $H^{-1}[E_0 - \epsilon, E_0 + \epsilon]$ translate into the local uniformity in E of the asymptotic expansion (114). The idea is to consider Υ as a distribution on the (s, E)-plane:

$$\Upsilon(s, E) = \sum_{k=0}^{\infty}\sum_j A_j(k)\,\varphi(k(E_j(k) - E))\,e^{iks}\,. \tag{151}$$

(This distribution is also of use in the study of the case when E is a critical value, see [3].) The analysis of (151) is analogous to that of Υ_E, so we will be brief. First, the operator

$$\mathcal{F}(u)(s,E) \;=\; \mathcal{F}_E(u)(s)$$

(where $\mathcal{F}_E$ is as in §4) is a Fourier integral operator given by the same oscillatory integrals (138). The canonical relation, $\mathcal{C}$, of $\mathcal{F}$ is the set of all points of the form

$$((s=\theta+tE,\kappa)\;,\;(\theta,\kappa\,;\,t,\kappa E\,;\,\overline{x}\,;\,\overline{x}))\;. \tag{152}$$

A version of Lemma 5.6 also holds for the derivatives of (124) with respect to E, and so the localization process of §4.2 can be applied to Υ. The conclusion is:

Proposition 6.3 *If g is such that $[E-\epsilon,E+\epsilon]\subset I_f$ and supp $f\subset g^{-1}(1)$, $\Upsilon=\mathcal{F}(\mathcal{K}_{f,g})$ modulo C^∞.*

Corollary 6.4 *The series (151) converges weakly to a distribution $\Upsilon(s,E)$ on the cylinder $S^1\times\mathbb{R}$ with wave-front set contained in the set of all $(s,E;\kappa,\lambda)$ such that there exists $(x,p)\in T^*M$ satisfying*

$$\left\{\begin{array}{ccl} \kappa\neq 0 & & \textit{and}\quad t:=\lambda/\kappa\in \textit{supp}\hat{\varphi}\\ \phi_t(x,p) &=& (x,p)\\ H(x,p) &=& E\\ s &=& \oint pdq \end{array}\right. \tag{153}$$

where the integral is along the periodic trajectory defined by (x,p) and t.

Notice that the inverse of the slope λ/κ of a covector in $\mathrm{WF}(\Upsilon)$ has the interpretation of the *period* of the classical trajectory with energy E producing the singularity.

Next we turn to the clean intersection condition that will ensure that Υ is a Lagrangian distribution.

Proposition 6.5 *Υ is a Lagrangian distribution when restricted to the open set $S^1\times(E_0-\epsilon,E_0+\epsilon)$ provided that:*

(1) The set

$$\mathcal{P}\;:=\;\{(z\,;\,t)\in H^{-1}(E_0-\epsilon,E_0+\epsilon)\times J\,;\,\phi_t(z)=z\}\;,$$

where J is some open neighborhood of $Supp\hat{\varphi}$ and $\{\phi_t\}$ the Hamilton flow of H on T^*M, is a submanifold, and

(2) $\forall(z,t)\in\mathcal{P}$, the tangent space $T_{(z,t)}\mathcal{P}$ equals the space of all $(\zeta,\tau)\in T_{(z,t)}(T^*M\times\mathbb{R})$ such that

$$\tau\Xi_z\;+\;d(\phi_t)_z(\zeta)\;=\;\zeta, \tag{154}$$

PROOF Recall the following basic theorem of FIO theory (see for example [25] Vol. IV). Let $\mathcal{F}$ be an FIO from a manifold Y to a manifold Z, and let $\Gamma\subset T^*Y\backslash\{0\}$ be a closed conic Lagrangian submanifold. The condition for $\mathcal{F}(u)$ to be Lagrangian, where $\mu\in I^{\cdot}(Y,\Gamma)$, is that the canonical relation of $\mathcal{F}$, $\mathcal{C}\subset(T^*Y\backslash\{0\})\times(T^*Z\backslash\{0\})$, intersects $\Gamma\times(T^*Z\backslash\{0\})$ cleanly. In the present case,

$$Y\;=\;S^1\times\mathbb{R}\times M\times M,\qquad Z\;=\;X^1\times\mathbb{R}$$

and one can easily show (as in [19]) that this condition is equivalent to the clean intersection of the immersed manifolds

$$\begin{array}{ccc} & & T^*M\times J\\ & & \downarrow\Phi\\ T^*M\times T^*\mathbb{R} & \hookrightarrow & T^*M\times T^*M\times T^*\mathbb{R} \end{array} \tag{155}$$

where

$$\Phi(z,t)\;=\;(z\,;\,\phi_t(z)\,;\,t,H(z))$$

and the horizontal arrow is the diagonal inclusion. This condition is precisely (1) and (2) in the Theorem.

□

It is straightforward that this condition implies the clean intersection conditions on the energy shell $H^{-1}(E)$ for all $E \in [E_0 - \epsilon, E_0 + \epsilon]$. Moreover, the clean intersection condition implies that the manifolds of periodic trajectories on $H^{-1}(E)$ depend smoothly on E. With this in mind, we can state:

Theorem 6.6 *The coefficients of the asymptotic expansion of (104) at every $E \in [E_0 - \epsilon, E_0 + \epsilon]$ depend smoothly on E, and the expansion is uniform in E.*

The proof is completely analogous to that of Theorem 6.3 in [37].

6.3 The periodic case.

We consider here the case when E is a regular value of H and the Hamilton flow of H on Σ_E is simply periodic with smallest period normalized to 2π.

Theorem 6.7 *There exist constants $C_1 > 0$, $C_2 > 0$ such that*

$$\{\, j\,;\, |E_j(\hbar) - E - \hbar\pi\sigma/2T| \leq C_1\hbar \,\} \subset \{\, j\,;\, |E_j(\hbar) - E - \hbar\pi\sigma/2T| \leq C_2\hbar^2 \,\}\,. \tag{156}$$

This is a clustering result: eigenvalues that are $\hbar$-close to E are actually $\hbar^2$ close. The second result is a geometric description of the asymptotic distribution of the eigenvalues in these clusters. Let $B = \Sigma_E/S^1$, where the action of S^1 on Σ_E is by the Hamilton flow of H. Then B is a smooth manifold (the manifold of trajectories), and it inherits a symplectic structure.

Theorem 6.8 *There is a smooth function, $\rho : B \to \mathbb{R}$, such that $\forall f \in C_0^\infty(\mathbb{R})$*

$$\frac{1}{\# J} \sum_{j \in J} f\left(\frac{E_j(\hbar) - E}{\hbar^2}\right) \sim \frac{1}{LVol(B)} \int_B f \circ \rho \, d\lambda_B \tag{157}$$

where J is the set on the right-hand side of (156), $LVol(B)$ is the Liouville measure of B and $d\lambda_B$ the Liouville density.

The proofs are a straightforward generalization of the corresponding statements in [2], working with the operator P_f of §4.

A Appendix A: Semi-classical ΨDOs on Manifolds.

We now discuss scFIOs in the case $M_1 = M_2 = M$ and Γ the diagonal. The corresponding scFIOs will be called *semi-classical pseudodifferential operators*, or scΨDO . Our goal is to associate, to certain functions a on T^*M, a scΨDO with principal symbol a.

Pseudodifferential operators with a small parameter, $a(x, \hbar D_x)$, are usually set up on $\mathbb{R}^n$, within the Weyl calculus, under the name of $\hbar$-admissible operators ([24], [26]). They differ from the usual ΨDO theory by the lack of homogeneity of the symbol: The principal symbol of $a(x, \hbar D_x)$ is the full amplitude of $a(x, D_x)$. On manifolds, ΨDO theory is well established by the classical result on the invariance of the symbol classes under coordinate changes, and the invariance of the principal symbol as a function on the cotangent bundle. The latter fails for the lower order terms of the symbol and this does not allow a naive definition of operators of semi-classical type. In this appendix we make explicit the theory of semi-classical ΨDOs on manifolds, within the framework used for the scFIOs of §3. After writing a direct definition of such operators we prove an Egorov type theorem. Finally we apply this machinery to prove the uniform distribution of eigenfunctions in case the classical flow is ergodic, that is the manifold version of the Theorem of Helffer, Martinez and Robert in [23].

A.1 Definitions and first properties

Let M be a smooth compact manifold, and let P be a classical, properly-supported pseudodifferential operator of order zero on $M \times \mathbb{R}$. (Recall that "properly supported" means that the projections from the support of the Schwartz kernel of P to $M \times \mathbb{R}$ are proper.) Therefore P, defined originally on $C_0^\infty(M \times \mathbb{R})$, extends to $C^\infty(M \times \mathbb{R})$. Denoting the variable on $\mathbb{R}$ by θ, we also assume that P commutes with D_θ.

Definition A.1 *For every $\hbar > 0$, define the operator $P_\hbar$ on $C^\infty(M)$ by:*

$$P_\hbar(f) \;=\; e^{-i\hbar^{-1}\theta}\, P[e^{i\hbar^{-1}\theta} f]\,. \tag{158}$$

The family $\{P_\hbar\}_\hbar$ will be called a scΨDO . If σ_P denotes the principal symbol of P, the sc symbol of $\{P_\hbar\}_\hbar$ is defined as the function

$$H_P(x,p) \;=\; \sigma_P(x, \xi = p, \kappa = 1)\,. \tag{159}$$

Remarks.

1.- Since $[P, D_\theta] = 0$ the right-hand side of (158), as well as σ_P, are independent of θ.

2.- The reason to insist that P be of order zero is because, morally speaking, in $P_\hbar$ every derivative should be accompanied by a factor of $\hbar$, and the latter have virtual degree (-1).

3.- Observe that according to our definition a Schrödinger operator

$$-\hbar^2\Delta + V$$

is *NOT* a scΨDO . However it becomes one after micro-localization in an energy band (i.e. the Fourier components of the operator P_f of §4 is a scΨDO). As we have already seen, such energy-localized operators are the only ones that have a reasonable semi-classical behavior.

4.- It is immediate that the class of scΨDO s forms an algebra, and that the standard symbol calculus formulae apply to the sc symbol.

We next obtain the local oscillatory integral representations of a scΨDO .

Proposition A.2 *If $\{P_\hbar\}$ is a scΨDO , then on functions f supported in a fixed compact in a coordinate chart of M $P_\hbar$ has the form*

$$P_\hbar(f) \;=\; \int e^{i\hbar^{-1}p\cdot x}\, \hat{f}(\hbar^{-1}p)\, a(x, h^{-1}p, h^{-1})\, dp \tag{160}$$

modulo $O(\hbar^\infty)$ in the C^∞ topology. Here $a(x,\xi,\kappa)$ is a classical symbol of order zero.

PROOF Since P commutes with D_θ, its Schwartz kernel $\mathcal{K}(x,\theta,y,\theta')$ is a distributional function of $(x, y, \theta - \theta')$. More precisely, just as in Lemma 3.1, $\mathcal{K}$ is of the form

$$\mathcal{K}(x,\theta,y,\theta') \;=\; \mathcal{K}_0(x,y,\theta-\theta')$$

where $\mathcal{K}_0$ is a Lagrangian distribution on $M \times M \times \mathbb{R}$ associated with the Lagrangian submanifold

$$\{\,(x, y = x, \theta = 0\,;\, \xi, -\xi, \kappa)\,\}\,. \tag{161}$$

Furthermore, since P is properly supported $\mathcal{K}_0$ is compactly supported. Therefore $\mathcal{K}$ is a *finite* sum of distributions of the form

$$\mathcal{K}_\alpha(x,\theta,y,\theta') \;=\; \int e^{i[\xi\cdot(x-y)+\kappa(\theta-\theta')]}\, A(x, y, \theta-\theta'; \xi, \kappa)\, d\xi\, d\kappa\,, \tag{162}$$

where each integral is supported in a local coordinate patch of the form $U \times U$ (where U is a coordinate patch on $M \times \mathbb{R}$) and A is a classical symbol of order zero. Applying e.g. Theorem 3.2. in [36] we see that we can write (162) in the form

$$\mathcal{K}_\alpha(x,\theta,y,\theta') \;=\; \int e^{i[\xi\cdot(x-y)+\kappa(\theta-\theta')]}\, a(x; \xi, \kappa)\, d\xi \quad \mathrm{mod}\, C^\infty\,, \tag{163}$$

in the support of $\mathcal{K}_\alpha$ (here a is another classical symbol of order zero). Let $f \in C^\infty(M)$; then, by the above, $P_\hbar(f)$ is a finite sum of integrals of the form

$$e^{-i\hbar^{-1}\theta} \int e^{i[(x-y)\cdot\xi+(\theta-\theta')\kappa]}\, e^{i\hbar^{-1}\theta'}\, f(y)\, a(x;\xi,\kappa)\, d\xi\, d\kappa\, dy \tag{164}$$

which, after the change of variables $\xi = \hbar p$, becomes the desired expression.

□

It is natural to ask which functions $b(x,p,\kappa)$ arise as amplitudes $b(x,p,\hbar^{-1}) = a(x,h^{-1}p,h^{-1})$ in (160). A first observation is that they must satisfy the following estimates: Given a compact K in x-space and given α,β,γ there is a $C>0$ such that $\forall x \in K$ and $\forall \kappa > 1$ one has

$$\left| D_\kappa^\alpha D_p^\beta D_x^\gamma\, b(x,p,\kappa)\right| \,\leq\, C\,\kappa^{-\alpha}\,(1+|p|^2)^{-|\beta|/2}\,. \tag{165}$$

Since a is a classical symbol an amplitude b has an asymptotic expansion of the form

$$b(x,p,\kappa) \,\sim\, \sum_{j=0}^{\infty} \kappa^{-j}\, b_j(x,p)$$

in the following sense: $\forall N>0\,,\,\alpha\,,\,\beta\,,\,\gamma\ \exists C$ such that $\forall\,\kappa > 1$

$$\left| D_\kappa^\alpha D_p^\beta D_x^\gamma \left(b(x,p,\kappa) - \sum_{j=0}^{N} \kappa^{-j}\, b_j(x,p)\right)\right| \leq C\,\kappa^{-\alpha-N-1}\,(1+|p|^2)^{-(|\gamma|+N+1)/2}\,. \tag{166}$$

$b_0(x,p)$ is the sc principal symbol. Furthermore, all functions b above have the property that the function $b(x,\xi/\kappa)$ extends to a smooth function away from $(\xi,\kappa)=(0,0)$. For our purposes the following converse is sufficient:

Definition A.3 *Given $U \subset \mathbb{R}^n$ open, define $\mathcal{S}^m(U)$ as the set of functions $b(x,p,\kappa) \in C^\infty(U \times \mathbb{R}^n \times \mathbb{R}^+)$ satisfying : $\forall \alpha,\ \beta,\ \gamma,\ N,\ K$ (K compact) $\exists C$ such that $\forall (x,p,\kappa) \in K \times \mathbb{R}^n \times (1,\infty)$*

$$\left|\, \partial_\kappa^\alpha\, \partial_p^\beta\, \partial_x^\gamma\, b(x,p,\kappa)\,\right| \,\leq\, C_{N,\alpha,\beta,\gamma}\,(1+|p|)^{-N}\,\kappa^{m-\alpha}\,. \tag{167}$$

Elements in $\mathcal{S}^m(U)$ are symbols in κ, uniformly Schwartz in p. We are interested in elements in $\mathcal{S}^0(U)$ having an expansion in decreasing powers of κ.

Definition A.4 *Let M be a smooth manifold. We denote by $\mathcal{S}(T^*M)$ the set of functions $H(x,p) \in C^\infty(T^*M)$ satisfying : $\forall\, N\ \exists C_N > 0$ such that*

$$|\,H(x,p)\,| \,\leq\, C_N\,(1+|p|)^{-N}\,, \tag{168}$$

where $|p|$ refers to an arbitrary Riemannian metric on M.

It is obvious that the class $\mathcal{S}$ is independent of the metric involved in (168). Elements in $\mathcal{S}$ are smooth functions uniformly Schwartz in the fiber direction of T^*M.

Lemma A.5 *Given $b \in C^\infty(U \times \mathbb{R}^n)$, $k^{-j}\, b(x,p) \in \mathcal{S}^{-j}(U)$ iff $b \in \mathcal{S}(T^*U)$.*

Definition A.6 *We define $\mathcal{S}_{\rm cl}(U)$ as the subset of all $b \in \mathcal{S}^m$ having an expansion of the form $b \sim \sum_{j=0}^\infty \kappa^{-j} b_j(x,p)$ where $\forall j\ b_j \in \mathcal{S}(T^*U)$, and the expansion as usual means that*

$$\forall N > 0 \quad b(x,p,\kappa) \,\equiv\, \sum_{j=0}^{N} k^{-j}\, b_j(x,p) \quad \mathit{mod}\ \mathcal{S}^{-N-1}\,.$$

Lemma A.7 *If $b \in \mathcal{S}_{\rm cl}(U)$, then the function a defined by:*

$$a(x;\xi,\kappa) \;=\; \begin{cases} 0 & \text{if}\,\kappa = 0\,, \\ b(x,\xi/\kappa,\kappa) & \text{if}\,\kappa \neq 0 \end{cases} \tag{169}$$

is a classical symbol of order zero (the fiber variables being (ξ,κ)). Moreover, a and each homogeneous term a_j in its asymptotic expansion vanishes to infinite order on $\Sigma := \{\kappa = 0\}$. Conversely, any classical symbol a of order zero with this vanishing property on Σ is asymptotic to one of the form (169).

Proof The derivatives $D_x^\alpha D_\xi^\beta D_\kappa^\gamma\, a$ are sums of terms of the form

$$\kappa^{-\gamma'} \xi^{\beta'} \tilde{b}(x,\xi/\kappa,\xi)\,,$$

where $\tilde{b}$ is some derivative of b. Since $b \in \mathcal{S}$, all such terms tend to zero as $\kappa \to \infty$ (provided that $\xi \neq 0$), we see that a is smooth on $U \times (\mathbb{R}^n \setminus \{0\}) \times \mathbb{R}^+$, vanishes to infinite order on Σ, and furthermore we obtain the following rough estimates on the derivatives:

$$\left| D_x^\alpha\, D_\xi^\beta\, D_\kappa^\gamma\, a(x,\xi,\kappa) \right| \leq C(1 + |\xi|^2 + \kappa^2)^\mu \tag{170}$$

where $\mu = \mu(\alpha,\beta,\gamma,K)$ with $x \in K$, (K compact).

Next, let $b \sim \sum_{j=0}^\infty \kappa^{-j}\, b_j$. Just as before, since $b_j \in \mathcal{S}(T^*U)$ the functions

$$a_j(x;\xi,\kappa) \;=\; \begin{cases} 0 & \text{if}\,\kappa = 0\,, \\ \kappa^{-j}\, b_j(x,\xi/\kappa) & \text{if}\,\kappa \neq 0 \end{cases}$$

are smooth on $U \times (\mathbb{R}^n \setminus \{0\}) \times \mathbb{R}^+$. They are clearly positive homogeneous in (ξ,κ) of degree $(-j)$. We now will use Proposition 3.6 in [36]: Given (170), to prove that a is a classical symbol it suffices to establish rough estimates of the form

$$\left| a(x,\xi,\kappa) - \sum_{j=0}^N a_j(x;\xi,\kappa) \right| \leq C_N\, (1 + |\xi|^2 + \kappa^2)^{\mu_N} \tag{171}$$

where $\mu_N \to -\infty$ as $N \to \infty$. This however is immediate from the assumption that $b \sim \sum_{j=0}^\infty \kappa^{-j}\, b_j$.

We now prove the converse. Thus let $a \sim \sum_{j=0}^\infty a_j$ be a classical symbol such that every a_j vanishes to infinite order on Σ. Define $\forall j$

$$b_j(x,p) \;=\; a_j(x,\xi = p, \kappa = 1)\,. \tag{172}$$

Observe that

$$b_j(x,p) \;=\; |p|^{-j}\, a_j(x, \frac{p}{|p|}, \frac{1}{|p|})$$

Since a_j vanishes to infinite order at Σ, b_j is in $\mathcal{S}(T^*U)$. Now let $b \in \mathcal{S}_{\rm cl}$ asymptotic to $\sum b_j$.

□

Lemma A.8 *The space of ΨDOs with amplitudes as in Lemma A.7 is a $*$ algebra under composition and transposition, and it's invariant under changes of coordinates of the form $(x,\theta) \mapsto (\Phi(x),\theta)$.*

Proof Indeed this is the algebra of amplitudes of ΨDOs on $M \times \mathbb{R}$ whose full symbol vanishes to all orders on Σ.

□

Definition A.9 *The algebra of scΨDO s on M defined by the previous Lemma will be called the algebra of admissible observables, and denoted $\mathcal{O}(M)$.*

Obviously the sc symbols of admissible observables are precisely the elements of $\mathcal{S}(T^*M)$. Finally, observe that an operator P on $M \times \mathbb{R}$ of giving rise to a scΨDO induces a ΨDO on $M \times S^1$ commuting with D_θ, the Fourier components of which are naturally identified with $P_\hbar$ with $\hbar = 1/m$.

A.2 Egorov's Theorem, positive quantization and uniformity of eigenfunctions.

Consider now the operator P_f of §4. Recall that it is a microlocalisation in a region $\mathcal{V}_I$ corresponding to an energy band I of an operator of the form $\sum_{j=1}^N h^j P_j$ where P_j is a differential operator of order j on M.

Theorem A.10 *(Egorov's theorem) If A_h is a scΨDO microlocally supported in $\mathcal{V}_I$ and with sc symbol $a(x,p)$, then*

$$e^{-itP_f^\hbar} A_\hbar \, e^{itP_f^\hbar}$$

is a scΨDO microlocally supported in $\mathcal{V}_I$ and with sc symbol $\phi_t^* a(x,p)$, where $\{\phi_t\}$ is the Hamilton flow of the symbol p of P.

Proof By the same arguments as in section 3,

$$e^{-itP_f^\hbar} A_\hbar \, e^{itP_f^\hbar} = e^{-i\hbar^{-1}\theta} e^{-itP_f} A_f \, e^{itP_f} e^{i\hbar^{-1}\theta} \tag{173}$$

By the classical Egorov theorem on $M \times S^1$, $e^{-itP_f} A \, e^{itP_f}$ is a zeroth order ΨDO with principal symbol $\Phi_t^* \tilde{a}$ where $\tilde{a}$ is the symbol of A, namely $a(x, \tau^{-1}\xi)$ and Φ_t is the Hamilton flow of the symbol of P_f (which we recall is $\tau p(x, \tau^{-1}\xi)$ on $\mathcal{V}_I$). The computations of §3 give the result.

□

Theorem A.11 *(On positive quantization.) Let $A_\hbar$ is a scΨDO with s.c.symbol $a \geq 0$. Then it exists an operator $\widehat{A}_\hbar$ such that:*
-$\widehat{A}_\hbar$ is a non-negative operator.
-$A_\hbar - \widehat{A}_\hbar = O(\hbar)$ in the topology of bounded operators in $L^2(M)$.

Proof By definition $A_\hbar = e^{-i\hbar^{-1}\theta} P e^{i\hbar^{-1}\theta}$, where P is a zeroth order pseudodifferential operator on $M \times \mathbb{R}$, commuting with D_θ. Then by the Friedrich quantization procedure (see [8]) one can find a non-negative $\widehat{P}$ such that $P - \widehat{P}$ is of order (-1). Since the Friedrich construction involves a pseudodifferential calculus with several frequency variables whose symbol is obtained from the symbol of P without altering the space variables, the symbol of $\widehat{P}$ doesn't depend of θ and so $\widehat{P}$ also commutes with D_θ. Define $\widehat{A}_\hbar$ by $\widehat{A}_\hbar = e^{-i\hbar^{-1}\theta} \widehat{P} e^{i\hbar^{-1}\theta}$. Since $D_\theta[P - \widehat{P}]$ is of order 0, $\hbar^{-1}[A_\hbar - A]$ is bounded.

□

With these ingredients at hand, the following result of Helffer, Martinez and Robert [23] extends immediately to manifolds:

Theorem A.12 *(Uniformity of eigenfunctions in the ergodic case.) Let $S_\hbar$ be as in §4. Let us suppose that the flow of H (the symbol of $S_\hbar$) is ergodic on a regular energy surface Σ_E. Then there exists a density one sequence of eigenvalues E_{j_k} of $S_\hbar$ tending to E as $\hbar$ tends to 0, such that for every sc observable $A_\hbar$ with sc symbol a one has:*

$$\lim_{\hbar \to 0} (\phi_{j_k}, A_\hbar \phi_{j_k}) = \int_{\Sigma_E} a(x,\xi) d\mu^L \tag{174}$$

where ϕ_{j_k} are the eigenfunctions corresponding to E_{j_k} and $d\mu^L$ is the Liouville measure on Σ_E.

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