A proof of the Gutzwiller Semiclassical Trace Formula using Coherent States decomposition

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Abstract

The Gutzwiller semiclassical trace formula links the eigenvalues of the Schrödinger operator $\widehat{H}$ with the closed orbits of the corresponding classical mechanical system, associated with the Hamiltonian H, when the Planck constant is small ("semiclassical régime"). Gutzwiller gave a heuristic proof, using the Feynman integral representation for the propagator of $\widehat{H}$. Later on mathematicians gave rigorous proofs of this trace formula, under different settings, using the theory of Fourier Integral operators and Lagrangian manifolds. Here we want to show how the use of coherent states (or gaussian beams) allows us to give a simple and direct proof.

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1 Introduction

Our goal in this paper is to give a simple proof of the "semiclassical Gutzwiller trace formula". The pioneering works in quantum physics of Gutzwiller [16] (1971) and Balian-Bloch [4] [5] (1972-74) showed that the trace of a quantum observable $\widehat{A}$, suitably localized in a spectral neighborhood of a given energy E for the quantum Hamiltonian $\widehat{H}$, can be expressed in terms of means of the classical observable A associated with $\widehat{A}$ over invariant sets for the classical flow corresponding to $\widehat{H}$ at energy E (energy surface, closed orbits...). In a sense this can be understood as a "correspondence principle" between classical and quantum mechanics as Planck's constant $\hbar$ goes to zero.

Between 1973 and 1975 several authors gave rigorous derivations of related results generalizing the classical Poisson summation formula from $\frac{d^2}{d\theta^2}$ on the circle to elliptic operators on compact manifolds: Colin de Verdière [8], Chazarain [7],Duistermaat-Guillemin [13]. The first article is based on a parametrix construction for the associated heat equation, while the second two replace this with a parametrix, constructed as a Fourier integral operator, for the associated wave equation. More recently, papers by Guillemin-Uribe (1989), Paul-Uribe (1991, 1995), Meinrenken (1992) and Dozias (1994) have developed the necessary tools from microlocal analysis in a non-homogeneous (semi-classical) setting to deal with Schrödinger-type Hamiltonians. Extensions and simplifications of these methods have been given by Petkov-Popov [30] and Charbonnel-Popov [6].

The coherent states approach presented here seems particularly suitable when one wishes to compare the phase space quantum picture with the phase space classical flow; furthermore it avoids problems with caustics, and the Maslov indices appear naturally. In short, it implies the Gutzwiller trace formula in a very simple and transparent way, without any use of the global theory of Fourier-integral operators and Lagrangian manifolds. In their place we use the coherent states approximation (gaussian beams) and the stationary phase theorem .

The use of gaussian wave packets is such a useful idea that one can trace it back to the very beginning of quantum mechanics, for instance, Schrödinger [34] (1926). However, the realization that these approximations are universally applicable, and that they are valid for arbitrarily long times, has developed gradually. Their history has also been complicated by the fact that, at least in the mathematical literature, they have never become textbook material. This has lead to their repeated rediscovery with a variety of different names, e.g. coherent states and gaussian beams. The first place that we have found where they are used in some generality is Babich [2] (1968) (see also [3]). Since then they have appeared, often as independent discoveries, in the work of Arnaud [1] (1973), Keller [23] (1974), Heller [19] (1975, 87), Ralston [32],[33] (1976,1982), Hagedorn [17] (1980-85), and Littlejohn [24] (1986) – and probably many more that we have not found. Their use in trace formulas was proposed by Wilkinson [35] (1987). The propagation formulas of [17] were extended in Combescure-Robert [10], with a detailed estimate on the error both in time and in Planck's constant. The early application of these methods in [2] was for the construction of quasi-modes, and this has been pursued further in [32] and Paul-Uribe [26]. There have also been recent applications to the pointwise behaviour of semiclassical measures [27].

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2 The Semiclassical Gutzwiller Trace Formula

We consider a quantum system in $L^2(\mathbb{R}^n)$ with Hamiltonian:

$$\widehat{H} = -\hbar^2\Delta + V(x), \tag{1}$$

where Δ is the Laplacian in $L^2(\mathbb{R}^n)$ and $V(x)$ a real, $C^\infty(\mathbb{R}^n)$ potential. The corresponding Hamiltonian for the classical motion is

$$H(q,p) = p^2 + V(q),$$

and for a given energy E $(\in \mathbb{R})$ we denote by Σ_E the "energy shell":

$$\Sigma_E := \left\{(q,p) \in \mathbb{R}^{2n} \ : \ H(q,p) = E\right\}. \tag{2}$$

More generally we shall consider Hamiltonians $\widehat{H}$ obained by the $\hbar$-Weyl quantization of the classical observable H, so we have $\widehat{H} = Op_\hbar^w(H)$.

$$Op_\hbar^w(H)\psi(x) = 2\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} H\left(\frac{x+y}{2}, \xi\right) \psi(y) \mathrm{e}^{\frac{i(x-y)\cdot\xi}{\hbar}} dy d\xi \tag{3}$$

where H is assumed to satisfy (H.0). An observable H is said to satisfy (H.0) if it is a C^∞-smooth, real valued function for $z = (x,\xi) \in \mathbb{R}^{2n}$, satisfying the following global estimates :

- (H.0) there exist non-negative constants C; C_γ such that

$$|\partial_z^\gamma H(z)| \leq C_\gamma < H(z) >, \ \ \forall z \in \mathbb{R}^{2n}, \ \forall \gamma \in \mathbb{N}^{2n} \tag{4}$$
$$< H(z) > \ \leq \ < H(z') >< z - z' >, \ \ \forall z, \ z' \in \mathbb{R}^{2n} \tag{5}$$

  where we have used the notation $< u > := (1 + |u|^2)^{1/2}$ for $u \in \mathbb{R}^m$.

Remark 2.1 *i) If the following estimate is satisfied*

$$|D^\gamma V(x)| \leq C_\gamma < x >^\delta \tag{6}$$

for some C_γ, and $\delta \in \mathbb{R}$, and for any multi-index $\gamma \in \mathbb{N}^n$; then $H(q,p) = p^2 + V(q)$ satisfies (H.0). *However, for Schrödinger operators we only need smoothness of the potential; no global assumptions at infinity are necessary when we restrict ourselves to a compact energy surface, assuming $E < \liminf_{|x|\to\infty} V(x)$. This can be proved using exponential decrease of the eigenfunctions [21].*
ii) The technical condition (H.0) *implies in particular that $\widehat{H}$ is essentially self-adjoint on $L^2(\mathbb{R}^n)$ for $\hbar$ small enough and that $\chi(\widehat{H})$ is a $\hbar$-pseudodifferential operator if $\chi \in C_0^\infty(\mathbb{R})$ (see [20]) .*

Let us denote by ϕ^t the classical flow induced by Hamilton's equations with Hamiltonian H , and by $S(q,p;t)$ the classical action along the trajectory starting at (q,p) at time $t=0$, and evolving during time t:

$$S(q,p;t) = \int_0^t (p_s \cdot \dot{q}_s - H(q,p))\, ds \tag{7}$$

where $(q_t, p_t) = \phi_t(q,p)$ We shall also use the notation: $\alpha_t = \phi_t(\alpha)$ where $\alpha = (q,p) \in \mathbb{R}^{2n}$, is a phase space point. Recall that a dot denotes derivation with respect to time.

An important role in what follows is played by the "linearized flow" around the classical trajectory, which is defined as follows. Let:

$$H''(\alpha_t) = \left.\frac{\partial^2 H}{\partial \alpha^2}\right|_{\alpha=\alpha_t} \tag{8}$$

be the Hessian of H at point $\alpha_t = \phi_t(\alpha)$ of the classical trajectory. Let J be the symplectic matrix

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{9}$$

where 0 and I are respectively the null and identity $n \times n$ matrices. Let $F(t)$ be the $2n \times 2n$ real symplectic matrix solution of the linear differential equation

$$\begin{cases} \dot{F}(t) = J\ H''(\alpha_t)\ F(t) \\ \\ F(0) = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} = I \end{cases} \tag{10}$$

$F(t)$ depends on $\alpha = (q,p)$, the initial point for the classical trajectory, α_t.

Let γ be a closed orbit on $\sum_E$ with period T_γ, and let us denote simply by F_γ the matrix $F_\gamma = F(T_\gamma)$. F_γ is usually called the "monodromy matrix" of the closed orbit γ. Of course, F_γ does depend on α, but its eigenvalues do not, since the monodromy matrix with a different initial point on γ is conjugate to F_γ. F_γ has 1 as eigenvalue of algebraic multiplicity at least equal to 2. In all that follows, we shall use the following definition:

Definition 2.2 *We say that γ is a nondegenerate orbit if the eigenvalue 1 of F_γ has algebraic multiplicity 2.*

Let σ denote the usual symplectic form on $\mathbb{R}^{2n}$:

$$\sigma(\alpha, \alpha') = p \cdot q' - p' \cdot q \qquad \alpha = (q,p);\ \alpha' = (q', p') \tag{11}$$

($\cdot$ is usual scalar product in $\mathbb{R}^n$). We denote by $\{\alpha_1, \alpha_1'\}$ the eigenspace of F_γ belonging to the eigenvalue 1, and by V its orthogonal complement in the sense of the symplectic form σ:

$$V := \left\{ v \in \mathbb{R}^{2n}\ :\ \sigma(v, \alpha_1) = \sigma(v, \alpha_1') = 0 \right\} \quad . \tag{12}$$

Then, the restriction P_γ of F_γ to V is called the (linearized) "Poincaré map" for γ.

We shall now assume the following. Let $(\Gamma_E)_T$ be the set of all periodic orbits on $\sum_E$ with periods T_γ, $0 < |T_\gamma| \leq T$ (including repetitions of primitive orbits and assigning negative periods to primitive orbits traced in the opposite sense).

- (H.1) There exists $\delta E > 0$ such that $H^{-1}([E - \delta E, E + \delta E])$ is a compact set of $\mathbb{R}^{2n}$ and E is a noncritical value of H (i.e. $H(z) = E \Rightarrow \nabla H(z) \neq 0$).
- (H.2) For any $T > 0$, $(\Gamma_E)_T$ is a discrete set, with periods $-T \leq T_{\gamma_1} < \cdots < T_{\gamma_N} \leq T$.
- (H.3) All γ in $(\Gamma_E)_T$ are nondegenerate, i.e. 1 is not an eigenvalue for the corresponding "Poincaré map", P_γ.
  We can now state the Gutzwiller trace formula. Let $\widehat{A} = Op_\hbar^w(A)$ be a quantum observable, such that A satisfies the following
- (H.4) there exists $\delta \in \mathbb{R}$, $C_\gamma > 0$ ($\gamma \in \mathbb{N}^{2n}$), such that
  $$|\partial_z^\gamma A(z)| \leq C_\gamma < z >^\delta \quad \forall z \in \mathbb{R}^{2n},$$
- (H.5) g a $\mathcal{C}^\infty$ function whose Fourier transform $\widehat{g}$ is of compact support with Supp $\widehat{g} \subset [-T, T]$
- and let χ be a smooth function with a compact support contained in $]E - \delta E, E + \delta E[$, equal to 1 in a neighborhood of E. Then the following "regularized density of states" $\rho_A(E)$ is well defined:

$$\rho_A(E) = \mathrm{Tr}\left(\chi(\widehat{H})\widehat{A}\chi(\widehat{H})g\left(\frac{E - \widehat{H}}{\hbar}\right)\right) \tag{13}$$

Note that (H.1) implies that the spectrum of $\widehat{H}$ is purely discrete in a neighborhood of E so that $\rho_A(E)$ is well defined. Then we have the following:

Theorem 2.3 *Assume* (H.0)-(H.3) *are satified for H,* (H.4) *for A and* (H.5) *for g. Then the following asymptotic expansion holds true, modulo $O(\hbar^\infty)$,*

$$\rho_A(E) \equiv (\pi)^{-n/2}\widehat{g}(0)\hbar^{-(n-1)}\int_{\Sigma_E} A(\alpha)d\sigma_E(\alpha) + \sum_{k\geq -n+2} c_k(\widehat{g})\hbar^k \tag{14}$$
$$+ \sum_{\gamma\in(\Gamma_E)_T}\left(2\pi)^{n/2-1}\{\widehat{g}(T_\gamma)\frac{e^{i(S_\gamma/\hbar+\sigma_\gamma\pi/2)}}{|\det(I - P_\gamma)|^{1/2}}\int_0^{T_\gamma^*}\frac{A(\alpha_s)}{|\nabla H|}ds + \sum_{j\geq 1} d_j^\gamma(\widehat{g})\hbar^j\right\}$$

where $A(\alpha)$ is the classical Weyl symbol of $\widehat{A}$,
T_γ^* is the primitive period of γ,
σ_γ is the Maslov index of γ ($\sigma_\gamma \in \mathbb{Z}$),
$S_\gamma = \oint_\gamma pdq$ is the classical action along γ,

$c_k(\widehat{g})$ *are distributions in* $\widehat{g}$ *with support in* $\{0\}$,
$d_j^\gamma(\widehat{g})$ *are distributions in* $\widehat{g}$ *with support* $\{T_\gamma\}$ *and* $d\sigma_E$ *is the Liouville measure on* $\sum_E$*:*

$$d\sigma_E = \frac{d\Sigma_E}{|\nabla H|} \qquad (d\Sigma_E \ \text{ is the Euclidean measure on } \Sigma_E)$$

Remark 2.4 *We can include more general Hamiltonians depending explicitly in* $\hbar$, $H = \sum_{j=1}^{j=K} \hbar^j H^{(j)}$ *such that* $H^{(0)}$ *satisfies* (H.0) *and for* $j \geq 1$,

$$|\partial^\gamma H^{(j)}(z)| \leq C_{\gamma,j} < H^{(0)}(z) > \tag{15}$$

It is useful for applications to consider Hamiltonians like $H^{(0)} + \hbar H^{(1)}$ *where* $H^{(1)}$ *may be, for example, a spin term. In that case the formula* (14) *is true with different coefficients. In particular the first term in the contribution of* T_γ *is multiplied by* $\exp\left(i \int_0^{T_\gamma^*} H^{(1)}(\alpha_s)|\dot{\alpha}|ds\right)$.

3 Preparations for the Proof

We shall make use of the "coherent states" which can be defined as follows. Let

$$\psi_0(x) = (\hbar\pi)^{-n/4} \ \exp\left(-\frac{|x|^2}{2\hbar}\right), \tag{16}$$

be the ground state of the n-dimensional harmonic oscillator, and for $\alpha = (q,p) \in \mathbb{R}^{2n}$,

$$\mathcal{T}(\alpha) = \exp\left\{\frac{i}{\hbar}(p \cdot x - q \cdot \hbar D_x)\right\} \tag{17}$$

is the Weyl-Heisenberg operator of translation by α in phase space where $D_x = \frac{\partial}{i\partial x}$ We also denote by

$$\varphi_\alpha := \mathcal{T}(\alpha)\psi_0 \tag{18}$$

the usual coherent states centered at the point α. Then it is known that any operator B with a symbol decreasing sufficiently rapidly is in trace class (see [14]), and its trace can be computed by

$$\mathrm{Tr}B = (2\pi\hbar)^{-n} \int < \varphi_\alpha, B\varphi_\alpha > d\alpha. \tag{19}$$

The regularized density of states $\rho_A(E)$ can now be rewritten as

$$\rho_A(E) = (2\pi)^{-n-1}\hbar^{-n} \int \widehat{g}(t) \ e^{iEt/\hbar} \ < \varphi_\alpha, \widehat{A}_\chi \, U(t) \ \varphi_\alpha > dtd\alpha \tag{20}$$

where $U(t)$ is the quantum unitary group :

$$U(t) = e^{-it\widehat{H}/\hbar} \tag{21}$$

and $\widehat{A}_\chi = \chi(\widehat{H})\widehat{A}\chi(\widehat{H})$.

Our strategy for computing the behavior of $\rho_A(E)$ as $\hbar$ goes to zero is first to compute the bracket

$$m(\alpha, t) =< \widehat{A_\chi}\varphi_\alpha, U(t)\varphi_\alpha >, \tag{22}$$

where we drop the subscript χ in A_χ for simplicity. It is useful to rewrite (16) as

$$\psi_0 = \Lambda_\hbar \widetilde{\psi}_0, \tag{23}$$

where $\Lambda_\hbar$ is the following scaling operator:

$$(\Lambda_\hbar \psi)(x) = \hbar^{-n/4}\ \psi\left(x\hbar^{-1/2}\right) \ \text{ and } \ \widetilde{\psi}_0(x) = \pi^{-n/4}\exp\left(-|x|^2/2\right) \quad . \tag{24}$$

First of all we shall use the following lemma, giving the action of an $\hbar$-pseudodifferential operator on a Gaussian.

Lemma 3.1 *Assume that A satisfies* (H.0). *Then we have*

$$\widehat{A}\varphi_\alpha = \sum_\gamma \hbar^{\frac{|\gamma|}{2}} \frac{\partial^\gamma A(\alpha)}{\gamma!} \Psi_{\gamma,\alpha} + O(\hbar^\infty) \tag{25}$$

in $L^2(\mathbb{R}^n)$, where $\gamma \in \mathbb{N}^{2n}$, $|\gamma| = \sum_1^{2n}$, $\gamma! = \prod_1^{2n}\gamma_j!$ and

$$\Psi_{\gamma,\alpha} = \mathcal{T}(\alpha)\Lambda_\hbar Op_1^w(z^\gamma)\widetilde{\psi}_0. \tag{26}$$

where $Op_1^w(z^\gamma)$ is the 1-Weyl quantization of the monomial :
$(x,\xi)^\gamma = x^{\gamma'}\xi^{\gamma''}$, $\gamma = (\gamma', \gamma'') \in \mathbb{N}^{2n}$.

This lemma is easily proved using a scaling argument and Taylor expansion for the symbol A around the point α. Thus $m(t,\alpha)$ is a linear combination of terms like

$$m_\gamma(\alpha, t) =< \Psi_{\gamma,\alpha}, U(t)\varphi_\alpha > . \tag{27}$$

Now we compute $U(t)\varphi_\alpha$, using the semiclassical propagation of coherent states result as it was formulated in Combescure-Robert [10]. We recall that $F(t)$ is a time dependent symplectic matrix (Jacobi matrix) defined by the linear equation (10). Met$F$ denotes the metaplectic representation of the linearized flow F (see for example Folland [14]), and the $\hbar$-dependent metaplectic representation is defined by

$$\mathrm{Met}_\hbar(F) = \Lambda_\hbar^{-1}\mathrm{Met}(F)\Lambda_\hbar \tag{28}$$

We will also use the notation

$$\delta(\alpha, t) = \int_0^t p_s \cdot \dot{q}_s ds - tH(\alpha) - \frac{p_t\cdot q_t - p\cdot q}{2} \tag{29}$$

From Theorem (3.5) of [10] (and its proof) we have the following propagation estimates in the L^2-norm: for every $N \in \mathbb{N}$ and every $T > 0$ it exists $C_{N,T}$ such that

$$\|U(t)\varphi_\alpha - \exp\left(\frac{i\delta(\alpha,t)}{\hbar}\right)\mathcal{T}(\alpha_t)\mathrm{Met}_\hbar(F(t))\Lambda_\hbar P_N(x,D_x,t,\hbar)\widetilde{\psi_0}\| \leq C_{N,T}\hbar^N \tag{30}$$

where $P_N(t,\hbar)$ is the $(\hbar,t)$-dependent differential operator defined by

$$P_N(x,D_x,t,\hbar) = I + \sum_{(k,j)\in I_N} \hbar^{k/2-j} p^w_{kj}(x,D,t)$$
$$\text{with } I_N = \{(k,j)\in \mathbb{N}\times\mathbb{N},\ 1\leq j\leq 2N-1,\ k\geq 3j,\ 1\leq k-2j<2N\} \tag{31}$$

where the differential operators $p_{kj}(x,D_x,t)$ are products of j Weyl quantization of homogeous polynomials of degree k_s with $\sum_{1\leq s\leq j} k_s = k$ (see [10] Theorem (3.5) and its proof). So that we get

$$p^w_{kj}(x,D_x,t)\widetilde{\psi_0} = Q_{kj}(x)\widetilde{\psi_0}(x) \tag{32}$$

where $Q_{kj}(x)$ is a polynomial (with coefficients depending on (α,t)) of degree k having the same parity as k. This is clear from the following facts: homogeneous polynomials have a definite parity, and Weyl quantization behaves well with respect to symmetries: $Op^w(A)$ commutes to the parity operator $\Sigma f(x) = f(-x)$ if and only if A is an even symbol and anticommutes with Σ if and only if A is an odd symbol) and $\widetilde{\psi_0}(x)$ is an even function. So we get

$$\begin{aligned} m(\alpha,t) = &\sum_{(j,k)\in I_N;|\gamma|\leq 2N} c_{k,j,\gamma}\hbar^{\frac{k+|\gamma|}{2}-j}\exp\left(\frac{i\delta(\alpha,t)}{\hbar}\right)\cdot \\ &\cdot\left\langle \mathcal{T}(\alpha)\Lambda_\hbar Q_\gamma\widetilde{\psi_0}, \mathcal{T}(\alpha_t)\Lambda_\hbar Q_{k,j}\mathrm{Met}(F(t))\widetilde{\psi_0}\right\rangle + O(\hbar^N) \end{aligned} \tag{33}$$

where $Q_{k,j}$ respectively Q_γ are polynomials in the x variable with the same parity as k respectively $|\gamma|$. This remark will be useful in proving that we have only entire powers in $\hbar$ in (14), even though half integer powers appear naturally in the asymptotic propagation of coherent states. By an easy computation we have

$$\begin{aligned} &\left\langle \mathcal{T}(\alpha)\Lambda_\hbar Q_\gamma\widetilde{\psi_0}, \mathcal{T}(\alpha_t)\Lambda_\hbar Q_{k,j}\mathrm{Met}(F(t))\widetilde{\psi_0}\right\rangle = \\ &\exp\left(-i\frac{1}{2\hbar}\sigma(\alpha,\alpha_t)\right)\left\langle \mathcal{T}_1\left(\frac{\alpha-\alpha_t}{\sqrt{\hbar}}\right)Q_\gamma\widetilde{\psi_0}, Q_{k,j}\mathrm{Met}(F(t))\widetilde{\psi_0}\right\rangle \end{aligned} \tag{34}$$

where $\mathcal{T}_1(\cdot)$ is the Weyl translation operator with $\hbar = 1$.
We set

$$m_{k,j,\gamma}(\alpha,t) = \left\langle \mathcal{T}_1\left(\frac{\alpha-\alpha_t}{\sqrt{\hbar}}\right)Q_\gamma\widetilde{\psi_0}, Q_{k,j}\mathrm{Met}(F(t))\widetilde{\psi_0}\right\rangle \tag{35}$$

$$m_0(\alpha,t) = \left\langle \mathcal{T}_1\left(\frac{\alpha-\alpha_t}{\sqrt{\hbar}}\right)\widetilde{\psi_0}, \mathrm{Met}(F(t))\widetilde{\psi_0}\right\rangle \tag{36}$$

We compute $m_0(\alpha, t)$ first. We shall use the fact that the metaplectic group transforms Gaussian wave packets into Gaussian wave packets in a very explicit way. If we denote by A, B, C, D the four $n\times n$ matrices of the block form of $F(t)$:

$$F(t) = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{37}$$

it is clear, since F is symplectic, that $U = A + iB$ is invertible. So we can define

$$M = VU^{-1}, \text{ where } V = (C + iD). \tag{38}$$

We have ([14], Ch.4)

$$m_0(\alpha, t) = (\det U)_c^{-1/2}\pi^{-n/2}\cdot$$
$$\cdot\int_{\mathbb{R}^n} \exp\left\{\frac{i}{2}(M+iI)x\cdot x) - \frac{i}{\sqrt{\hbar}}(x - \frac{q-q_t}{2})\cdot(p-p_t+i(q-q_t))\right\} dx \tag{39}$$

Remark 3.2 *In (39), $(z(t))_c^{1/2}$ has the following meaning :*
if $t\mapsto z(t)$ is a continuous mapping from $\mathbb{R}$ into $\mathbb{C}\backslash\{0\}$ such that $z(0) > 0$ then $(z(t))_c^{1/2}$ denotes the square root defined by continuity in t starting from $\sqrt{z(0)} > 0$. To avoïd confusion we shall use later the following notation, for $z \in \mathbb{C}\backslash\{0\}$,

$$(z)_*^{1/2} = |z|^{1/2}\mathrm{e}^{iarg(z)/2}, \text{ where } 0 \le arg(z) < 2\pi.$$

More generally we can easily see that $m_{k,j,\gamma}(\alpha, t)$ is a linear combination of the following integrals, where $\gamma \in \mathbb{N}^n$,

$$I(\gamma,\zeta) = \int_{\mathbb{R}^n} x^\gamma \exp\left(\frac{i}{2}(M+iI)x\cdot x\right)\exp\left(-ix\cdot\frac{\zeta}{\sqrt{\hbar}}\right) dx \tag{40}$$

Using classical results on the Fourier transform of Gaussians functions, we get, for $\gamma = 0$,

$$I(0,\zeta) = (2\pi)^{n/2}\left(\det(I - iM)\right)_c^{-1/2}\exp\left(\frac{i}{2\hbar}(M+iI)^{-1}\zeta\cdot\zeta\right). \tag{41}$$

Hence for every γ, we get

$$I(\gamma,\zeta) = R_\gamma\left(\frac{\zeta}{\sqrt{\hbar}}\right) I(0,\zeta) \tag{42}$$

where R_γ is a polynomial of degree $\le |\gamma|$ with the same parity as $|\gamma|$.
So the above calculus shows that, up to arbitrary large power of $\hbar$, $m(\alpha, t)$ is a polynomial in $(\hbar, \hbar^{-1})$, where the coefficients of the negative power of $\hbar$ are vanishing for $\alpha = \alpha_t$,

$$m(\alpha, t) \equiv \sum_{(k,k_1,s,j)\in J_N} \hbar^{\frac{k+k_1-s}{2}-j} b_{k,k_1,s,j}(\alpha, t)\exp\left(\frac{1}{\hbar}\Phi(\alpha, t)\right), \tag{43}$$

where

$$J_N := \{(k, k_1, s, j) \in \mathbb{N}^4,\ (k, j) \in I_N,\ 0 \le s \le k + k_1,\ k + k_1 - s \in 2\mathbb{N}\}$$

$$\begin{aligned}\Phi(\alpha, t) = iS(\alpha; t) &+ \frac{i}{2}(q \cdot p - q_t \cdot p_t + p_t \cdot q - q_t \cdot p) \\ &-\frac{1}{4}|\alpha - \alpha_t|^2 + \frac{1}{4}(\alpha - \alpha_t) \cdot W(\alpha - \alpha_t)\end{aligned} \tag{44}$$

where $\cdot$ denotes the usual bilinear product in $\mathbb{C}^n$, and α (resp. α_t) denotes $q+ip$ (resp. q_t+ip_t) and

$$W(t) = (I + iM(t))(I - iM(t))^{-1}. \tag{45}$$

Moreover, for every $s \ge 1$, $b_{k,k_1,s,j}(\alpha, t)$ **vanishes for** $\alpha = \alpha_t$ **to order** $\ge s$.
We can compute $a_0(\alpha, t) := b_{2,0,0,1}(\alpha, t)$, the principal term of $m(\alpha, t)$. We have

$$a_0(\alpha, t) = (2\pi)^{n/2} \left(\det \frac{Y}{2}\right)_c^{-1/2} A(\alpha) \tag{46}$$

where $Y = U - iV$.

Our next step is to show that the stationary phase method (Hörmander [22]) in variables (α, t) can be performed with the complex phase $iEt + \Phi(\alpha, t) =: \Phi_E(\alpha, t)$, assuming some propertiies on the classical flow ϕ^t. This will be done in the next section. Note that the contribution of $t = 0$, $\alpha \in \Sigma_E$ gives the "Weyl terms" (first line in the RHS of (14). The computation of this term by this method (coherent states) was done in [9].

4 Stationary Phase Computations

¿From the previous section one sees that (14) will be a consequence of asymptotic expansion as $\hbar$ goes to 0 of Fourier integrals of the following type

$$I(E, \hbar) = \int_{\mathbb{R}_t \times \mathbb{R}^{2n}_\alpha} a(\alpha, t) e^{\frac{i}{\hbar}(tE - i\Phi(\alpha,t))} dt d\alpha, \tag{47}$$

where the complex phase Φ is computed in the previous section, and a is a smooth amplitude with compact support in $\mathbb{R}_t \times \mathbb{R}^{2n}_\alpha$.

We recall the following notation for use later: $U = A + iB$, $V = C + iD$, and $Y = U - iV$, $Z = U + iV$. Then

$$W(t) = Z(t)Y(t)^{-1} = (I + iM(t))(I - iM(t))^{-1}, \tag{48}$$

where $M(t) = VU^{-1}$. Since F is symplectic, the matrix M is symmetric with positive imaginary part, and hence $||W(t)|| < 1$.

The function Φ satisfies $\Re(\Phi) \le 0$ and we have

$$\{\Re(\Phi) = 0\} \iff \{\alpha = \alpha_t\}.$$

This follows from (44), since $||W(t)|| < 1$. We wish to apply the stationary phase method to expand $I(E, \hbar)$. We will apply the following variant of the stationary phase theorem with complex phase ([22], Vol.1, Theorem(7.7.5)).

Theorem 4.1 (stationary phase expansion) *Let $\mathcal{O} \subset \mathbb{R}^d$ be an open set, and let $a, f \in C^\infty(\mathcal{O})$ with $\Im f \geq 0$ in $\mathcal{O}$ and supp $a \subset \mathcal{O}$. We define*

$$M := \{x \in \mathcal{O},\ \Im f(x) = 0,\ f'(x) = 0\},$$

and assume that M is a smooth, compact and connected submanifold of $\mathbb{R}^d$, of dimension k, such that, for all $x \in M$, the hessian $f''(x)$ of f is nondegenerate on the normal space N_x to M at x.

Under the conditions above, the integral $J(\omega) = \int_{\mathbb{R}^d} \mathrm{e}^{i\omega f(x)} a(x) dx$ has the following asymptotic expansion as $\omega \to +\infty$, modulo $O(\omega^{-\infty})$,

$$J(\omega) \equiv \left(\frac{2\pi}{\omega}\right)^{\frac{d-k}{2}} \sum_{j \geq 0} c_j \omega^{-j} \tag{49}$$

The coefficient c_0 is given by

$$c_0 = \mathrm{e}^{i\omega f(m_0)} \int_M \left[\det\left(\frac{f''(m)|_{N_m}}{i}\right)\right]_*^{-1/2} a(m) dV_M(m), \quad \text{(see remark(3.2))} \tag{50}$$

where $dV_M(m)$ is the canonical Euclidean volume in M, $m_0 \in M$ is arbitrary.

sketch of proof: Using a partition of unity, we can assume that $\mathcal{O}$ is small enough such that we have normal, geodesic coordinates in a neighborhood of M. So we have a diffeomorphism

$$\chi : \mathcal{U} \longrightarrow \mathcal{O},$$

where $\mathcal{U}$ is an open neighborhood of $(0,0)$ in $\mathbb{R}^k \times \mathbb{R}^{d-k}$, such that

$$\chi(x', x'') \in M \iff x'' = 0$$

and if $m = \chi(x', 0) \in M$ we have

$$\chi'(x', 0)(\mathbb{R}^k_{x'}) = T_m M \tag{51}$$

$$\chi'(x', 0)(\mathbb{R}^{d-k}_{x''}) = N_m M, \quad \text{(normal space at } m \in M) \tag{52}$$

So the change of variables $x = \chi(x', x'') = x$ gives the integral

$$J(\omega) = \int_{\mathbb{R}^d} \mathrm{e}^{i\omega f(\chi(x', x''))} a(x', x'') |\det \chi'(x', x'')| dx' dx'' \tag{53}$$

The phase $\tilde{f}(x', x'') := f(\chi(x', x''))$ satisfies obviously

$$\left\{\tilde{f}'_{x''}(x', x'') = 0,\ \Im \tilde{f}(x', x'') = 0\right\} \iff x'' = 0 \tag{54}$$

Hence, we can apply the stationary phase Theorem (7.7.5) of [22] (Vol.1), in the variable x'', to the integral (53), where x' is a parameter (the assumptions of [22] are satisfied, uniformly for x' close to 0). We remark that all the coefficients c_j of the expansion can be computed using the above local coordinates and Theorem (7.7.5) of [22]. ∎

The phase $\Phi_E(\alpha,t) = \Phi(\alpha,t) + itE$ is critical on the set

$$\mathcal{C}_E = \{(t,\alpha) \in \mathbb{R}_t \times \mathbb{R}^{2n}, \ \ \alpha_t = \alpha, \ H(\alpha) = E\}.$$

$\mathcal{C}_E$ being a bounded set, a classical non stationary phase argument shows that it is sufficient to assume that the amplitude a has a compact support.
We will assume now that

$$\mathcal{C}_E = (\{0\} \times \Sigma_E) \cup \{\gamma_1, \cdots, \gamma_N\} \tag{55}$$

where $\{\gamma_1, \cdots, \gamma_N\}$, is a finite set of nondegenerate closed orbits with periods $\{T_{\gamma_1}, \cdots, T_{\gamma_N}\}$. For simplicity we take $N = 1$. The general case follows easily by a partition of unity: it is sufficient to consider the case when the support of $a(\alpha,t)$ is small enough and contains one orbit γ_E on the energy level Σ_E of period T_E. Hence the support of $a(\alpha,t)$ is in a small neighborhood of $\gamma_E \times \{T_E\}$. Under our assumption, 1 is an eigenvalue of $F(T_E)$ of multiplicity 2. By Poincaré's Continuation Theorem this implies that for $\hat{E}$ near E the critical set consists of an isolated periodic orbit $\gamma_{\hat{E}}$ with period $T_{\hat{E}}$, a smooth function of $\hat{E}$. To be more explicit let us recall the following construction in a neighborhood $\mathcal{V}$ of a fixed point $\alpha_0 \in \gamma_E$. Using the Hamiltonian straightening theorem (see [18]) we can construct a smooth function $\mathcal{A}$ such that $\{H, \mathcal{A}\} = 1$ in $\mathcal{V}$. So that $\{\mathcal{A} = 0\} \cap \mathcal{V} := \mathcal{N}$ defines a Poincaré section for γ. The return time map T is defined by the implicit function theorem applied to $\mathcal{A}(\Phi^{T(\alpha)}(\alpha)) = 0$ and the Poincaré map $\mathcal{P}_\gamma : \mathcal{V} \to \mathcal{N}$ by

$$\mathcal{P}_\gamma(\alpha) = \phi^{T(\alpha)}(\alpha)$$

In $\mathcal{V}$ we get new symplectic coordinates by setting $\alpha = \alpha(e,f,\nu)$, where $\mathcal{A}(\alpha) = f$, $H(\alpha) = e$, $\nu \in \mathbb{R}^{2(n-1)}$; $\alpha_0 = \alpha(E,0,0)$. Moreover, using that γ_E is non degenerate, we see that $\mathcal{N} \cap \mathcal{C}_e = \{\alpha_e\}$ for e close to E, where α_e is smooth in e and such that $\alpha_E = \alpha_0$. So we have a basis of generalized eigenvectors for the eigenvalue 1 of the monodromy matrix $F := F(T_E)$

$$(F - I)\dot{\alpha} \ = \ 0 \tag{56}$$

$$(F - I)\alpha'_E \ = \ T'_E\dot{\alpha} \tag{57}$$

where f'_E is the derivative of f in the energy variable e evaluated at E.
Note that we have

$$\alpha'_E = -J\nabla\mathcal{A}(\alpha_0)$$

We set

$$W^\sharp(t) = \begin{pmatrix} W(t) & -iW(t) \\ -iW(t) & -W(t) \end{pmatrix}, \quad G = \frac{1}{2}(W^\sharp(t) - I).$$

The first derivatives of Φ_E in the variables (α,t), modulo $O(|\alpha_t - \alpha|^2)$, are given by the following formulas in which we use $\tilde{X}$ to denote the transpose of the matrix X,

$$
\begin{aligned}
\frac{\partial \Phi_E}{\partial t} &= i\left(E - H(\alpha) - \frac{1}{2}(\alpha_t - \alpha)\cdot J\dot{\alpha}_t\right) + \frac{1}{2}W^\sharp(t)\dot{\alpha}_t \cdot (\alpha_t - \alpha) \\
\frac{\partial \Phi_E}{\partial \alpha} &= \frac{i}{2}(I + \tilde{F}(t))J(\alpha_t - \alpha) + \frac{1}{2}(\tilde{F}(t) - I)(W^\sharp(t) - I)(\alpha_t - \alpha). \qquad (58)
\end{aligned}
$$

The next step towards application of a stationary phase theorem is the computation of the Hessian matrix Φ'' of Φ on the critical set $\mathcal{C}_E$,

$$
\begin{aligned}
\frac{\partial^2 \Phi}{\partial t^2} &= G\dot{\alpha}\cdot\dot{\alpha} =: a \\
\frac{\partial^2 \Phi}{\partial t \partial \alpha} &= iJ\dot{\alpha} + (\tilde{F}(t) - I)G\dot{\alpha} =: \eta \\
\frac{\partial^2 \Phi}{\partial \alpha^2} &= \frac{i}{2}(JF(t) - \tilde{F}(t)J) + (\tilde{F}(t) - I)G(F(t) - I) =: L \qquad (59)
\end{aligned}
$$

Now we need to compute the determinant of the Hessian $\Phi''_{(T_E\alpha_0)}$ restricted to $\mathcal{E}$, the orthogonal complement of the tangent space to γ in $\mathbb{R}_t \times \mathbb{R}^{2n}_\alpha$. Since $\dot{\alpha}$ is an eigenvector for F with eigenvalue 1, $(0, \dot{\alpha})$ is a (real) vector in the null space of $\Phi''_{(T_E,\alpha_0)}$. Thus

$$
\det(\Phi''_{(T_E,\alpha_0)} \mid \mathcal{E}) = \det\begin{pmatrix} a & \eta \\ \eta & L + \Pi \end{pmatrix}, \qquad (60)
$$

where Π is the orthogonal projection on $\dot{\alpha}$. Using $\tilde{F}JF = J$, we find

$$
\begin{aligned}
L &= K(F - I) \\
\text{with} \quad K &= \tilde{F}(G + \frac{i}{2}J) - (G - \frac{i}{2}J) \qquad (61)
\end{aligned}
$$

To compute $\det K$ we use the definition of G to obtain

$$
\begin{aligned}
2K &= \tilde{F}\begin{pmatrix} W - I & -i(W - I) \\ -i(W + I) & -W - I \end{pmatrix} - \begin{pmatrix} W - I & -i(W + I) \\ -i(W - I) & -W - I \end{pmatrix}, \\
&= \begin{pmatrix} I & iI \\ 0 & I \end{pmatrix}\begin{pmatrix} 0 & N \\ -2iI & Q \end{pmatrix}\begin{pmatrix} I & 0 \\ iI & I \end{pmatrix} \qquad (62)
\end{aligned}
$$

where

$$
N = 2((\tilde{A} - i\tilde{B})M - \tilde{C} + i\tilde{D})(I - iM)^{-1}, \text{ and } R = 2(\tilde{B}M - \tilde{D} + I)(I - iM)^{-1}.
$$

Using $\tilde{F}JF = J$, one computes $((\tilde{A}-i\tilde{B})M-\tilde{C}+i\tilde{D})(A+iB) = 2iI$ and $(\tilde{B}M-\tilde{D})(A+iB) = -I$. Thus $N = 4iY^{-1}$ and $Q = 2(U - I)Y^{-1}$. Thus from (62) we have the following formulas for the determinant and the inverse of K

$$
\det K = (-1)^n \det\left(\frac{Y}{2}\right)^{-1} \qquad (63)
$$

$$K^{-1} = -\frac{1}{2}\begin{pmatrix} U-I & -i(I+U) \\ iI+V & -(I+iV) \end{pmatrix}, \text{i.e.}$$

$$K^{-1} = -\frac{1}{2}(F - I + i(F+I)J). \tag{64}$$

¿From (64) we compute

$$K^{-1}\dot{\alpha} = \frac{i}{2}(F+I)J\dot{\alpha}.$$

Thus $L + \Pi = KR$ where

$$R = F - I + \frac{i}{2}(F+I)J\Pi. \tag{65}$$

To proceed we will assume that the null space of $F-I$ is spanned by $\dot{\alpha}$ (i.e $T'_E \neq 0$). Thus, since the algebraic multiplicity of 1 as an eigenvalue for F is two, there is a (real) vector β such that $(F-I)\beta = \dot{\alpha}$, and we fix β by requiring $\beta \cdot \dot{\alpha} = 0$. So we have, using (61) and $\tilde{F}J\dot{\alpha} = J\dot{\alpha}$,

$$(L+\Pi)\beta = K(F-I)\beta = K\dot{\alpha} = \eta.$$

Hence

$$\det(\Phi''_{|\mathcal{E}}) = \det\begin{pmatrix} a - \beta\cdot\eta & \eta \\ 0 & L+\Pi \end{pmatrix}.$$

Computing $a - \beta \cdot \eta$ we get

$$a - \beta\cdot\eta = -i\beta\cdot J\dot{\alpha} = i\dot{\alpha}\cdot J\beta.$$

Note that $\beta \cdot J\dot{\alpha} = \sigma(\dot{\alpha}, \beta)$ is nonzero. At this point we have

$$\det(\Phi''_{|\mathcal{E}}) = (iJ\beta\cdot\dot{\alpha})(\det K)(\det R) \tag{66}$$

with $\det K$ given in (63), and it remains to compute $\det R$.

We will compute $\det R$ in an orthonormal basis $\{v_j\}_{1\leq j\leq 2n}$ for $\mathbb{R}^{2n}$ with $v_1 = (1/|\dot{\alpha}|)J\dot{\alpha}$ and $v_2 = (1/|\beta|)J\beta$. Letting $V = \text{span}\{v_j\}_{3\leq j\leq 2n}$, we have $v \in V$ if and only if $\sigma(v,\dot{\alpha}) = \sigma(v,\beta) = 0$. Thus V is a Poincaré section for the closed orbit γ, and $F_{|V}$ is the Poincaré map P_γ . Since $\tilde{F}JF = J$, one computes $\tilde{F}v_1 = v_1$ and $\tilde{F}v_2 = v_2 - (|\dot{\alpha}|/|\beta|)v_1$. Since we are using a real orthonormal basis, and hence the matrix of the transpose is the tranpose of the matrix, the matrix of $F - I$ in this basis has the form

$$F - I = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ -\frac{|\dot{\alpha}|}{|\beta|} & 0 & 0 & \cdots & 0 \\ a_3 & b_3 & & & \\ \vdots & \vdots & & P_\gamma - I & \\ a_{2n} & b_{2n} & & & \end{pmatrix}.$$

Let us compute the matrix R using (65).

$$R = \begin{pmatrix} 0 & w_2 & w_3 & \cdots & w_{2n} \\ 2c & cw_2 & cw_3 & \cdots & cw_{2n} \\ a_3 & b_3 + \frac{1}{2}w_2 a_3 & \star + \frac{1}{2}w_3 a_3 & \cdots & \star + \frac{1}{2}w_{2n} a_3 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{2n} & b_{2n} + \frac{1}{2}w_2 a_{2n} & \star + \frac{1}{2}w_3 a_{2n} & \cdots & \star + \frac{1}{2}w_{2n} a_{2n} \end{pmatrix}. \tag{67}$$

where $2c = -\frac{|\dot\alpha|}{|\beta|}$, $w_j = (\frac{i}{|\dot\alpha|})\dot\alpha \cdot v_j$ and $\star$ is the generic matrix element of $(F-I)|_V = P_\gamma - I$.

In the matrix (67), by subtracting of the first line from the other lines we compute

$$\det R = \det \begin{pmatrix} 0 & w_2 & w_3 & \cdots & w_{2n} \\ -\frac{|\dot\alpha|}{|\beta|} & 0 & 0 & \cdots & 0 \\ a_3 & b_3 & & & \\ \vdots & \vdots & & P_\gamma - I & \\ a_{2n} & b_{2n} & & & \end{pmatrix}. \tag{68}$$

Since $P_\gamma - I$ is invertible, there is $v \in V$ such that $(P_\gamma - I)v = \sum_{j=3}^{2n} b_j v_j$. Thus performing the appropriate column operations on the matrix in (68), we see

$$\det R = \frac{|\dot\alpha|}{|\beta|}\left(\frac{i\dot\alpha \cdot J\beta}{|\dot\alpha||\beta|} - \frac{i}{|\dot\alpha|}\dot\alpha \cdot v\right)\det(P_\gamma - I). \tag{69}$$

By construction $(F-I)v = (F-I)v_2$ which implies $v = v_2 + b\dot\alpha$. Using $v_2 \cdot v = 0$, one computes b, and finds

$$\dot\alpha \cdot v = \frac{\dot\alpha \cdot J\beta}{|\beta|} - \frac{|\dot\alpha|^2|\beta|}{\dot\alpha \cdot J\beta}.$$

Substituting this into (69) and substituting the resulting formula for $\det R$ in (66) gives the final result:

$$\boxed{\det(\Phi''_{|\mathcal{E}}) = (-1)^{n-1}\det\left(\frac{Y}{2}\right)^{-1}|\dot\alpha|^2\det(P_\gamma - I)} \tag{70}$$

This formula holds true when $T'_E = 0$ as well, for if $T'_E = 0$ then we can approach F by symplectic matrices F_ε such that 1 is a simple eigenvalue of F_ε with a non trivial 2×2 Jordan block. ∎

To finish the proof of (14) we apply the stationary phase theorem (4.1). In particular we can compute the first term of the contribution of T_γ. Using (46) and (70), we get,

$$d_0^\gamma = \hat g(T_\gamma)e^{iS_\gamma/\hbar}\int_\gamma \left[|\dot\alpha|^2\frac{(-1)^{1-n}\det(P_\gamma - I)}{\det\frac{Y}{2}}\right]_*^{-1/2}\left(\det\frac{Y}{2}\right)_c^{-1/2} AdV_\gamma(m) \tag{71}$$

Using $dV_\gamma(\alpha_s) = ds$ we get the result for d_0^γ.
We remark here that the Maslov index σ_γ is determined by (71) and our remark (3.2).
The others coefficients, d_j^γ, are spectral invariants which have been studied by Guillemin and Zelditch. In principle we can compute them using our explicit approach. ∎

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