Phase-Space Semiclassical Analysis. Around Semiclassical Trace Formulae

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Résumé

(1) What is semiclassical Analysis ?
(2) What is a Trace Formula ?
(3) Physical Motivations : "Quantum Chaos"
(4) Gutzwiller Trace Formula . (Rigorous Approach)

COURS ÉCOLE D' ÉTÉ de CARGÈSE

"CHAOTIC DYMNAMICS ; CLASSICAL AND QUANTUM TRANSPORT"

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CLASSICAL WORLD

$Z = \mathrm{R}^n \times \mathrm{R}^n$ PHASE SPACE

$z := (q, p)$ classical state of a particle

q : position or coordinate

p : momentum

Hamiltonian $H = \frac{p^2}{2m} + V(q)$

Real

Phase-Space Evolution : $(q, p) \to (q_t, p_t) = \phi_H^t(q, p)$

ϕ_H^t preserves Phase-Space volumes

Classical Observables

$A : Z \mapsto \mathrm{R}$

Evolution of classical Observables

$A \circ \phi_H^t$

Geometrical Tranformations

• Phase-space translations

•, $J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}$ represents rotations of $\frac{\pi}{2}$

• General **symplectic** tranformations, ie

QUANTUM WORLD

$\mathcal{H} = L^2(\mathrm{R}^n)$ Hilbert space of quantum states

$\varphi \in \mathcal{H}$ "wavefunction"

$\hat{Q}$

$\hat{P} := -i\hbar\nabla$ self-adjoint Operators

Quantum **Hamiltonian** $\hat{H} := -\frac{\hbar^2}{2m}\Delta + V(q)$

Self-Adjoint

Quantum evolution : $U_H(t) := e^{-it\hat{H}/\hbar}$
$\varphi \to \varphi_t := U_H(t)\varphi$

Unitary Operator

Quantum Observables

$\hat{A}$: Weyl Quantization of A

Evolution of Quantum Observables

$\hat{A}_t := U_H^*(t)\hat{A}U_H(t)$

Unitary Transformations in $\mathcal{H}$

• $\hat{T}(z) := \exp(i\hat{Z}.Jz/\hbar)$ Weyl-Heisenberg operator

• $\mathcal{F}$ Fourier Transformation

• General operators of **metaplectic** Group

CLASSICAL WORLD (continued)

Preserve symplectic form $\sigma(z, z') = z.Jz'$

M : **symplectic matrix** $2n \times 2n$

Example $M = \begin{pmatrix} e^{\gamma}\mathbb{1} & 0 \\ 0 & e^{-\gamma}\mathbb{1} \end{pmatrix}$
dilation/squeezing transformation

Multiplicative Group :
$M = M_1 M_2$ symplectic

CLASSICAL STATE
Point $z \in Z$

Probability Distribution
in PHASE SPACE :

$f: \ Z \mapsto \mathrm{R}^+$

$f(q, p) \geq 0$

$\int_Z dz f(z) = 1$

QUANTUM WORLD (continued)

$i\sigma(\hat{Z}, z)$ generator of Weyl-Heisenberg Group

$B: \ 2n \times 2n$ real symmetric
$M = e^{JB} \rightarrow \hat{R}(M) = e^{i\hat{Z}.B\hat{Z}/2\hbar}$

$\hat{D}(\gamma) := \exp \frac{i\gamma}{2\hbar}(\hat{Q}.\hat{P} + \hat{P}.\hat{Q}))$

$\hat{R}(M_1 M_2) = \hat{R}(M_1)\hat{R}(M_2)$ is **Group**

COHERENT STATE $|z\rangle$

WIGNER, HUSIMI distributions

$\varphi \in \mathcal{H}, \ \|\varphi\| = 1$

Wigner Distribution

$\rightarrow W_\varphi(q, p)$
not ≥ 0 in general

Husimi Distribution

$H_\varphi(z) := |\langle\varphi|z\rangle|^2 \geq 0$

$\int_Z dz W_\varphi(z) = \int_Z dz H_\varphi(z) = 1$

1 What is Semiclassical Analysis ?

Semiclassical Analysis is the passage to the Limit $\hbar \to 0$ in the Quantum description in terms of the Evolution of states or Observables. It allows to better understand how the classical world description arises from a Quantum Reality.

However the limit $\hbar \to 0$ is a SINGULAR one, and in particular doesn't commute with the limit of large times $t \to \infty$, where classically long term UNPREDICTIBILITY ("chaos") manifests itself.

It will appear in what follows that Semiclassical Analysis (mathematical/physical) has to deal with estimates of Highly Oscillating Integrals with Small Parameter $\hbar$.

In what follows we shall present an illustration of Semiclassical Analysis which is simply an estimate of the Semiclassical Propagation of the so-called **coherent states** using the material presented in the comparative tableau above. The coherent states, usually denoted φ_z in the mathematical notation, or $|z\rangle$ in the Dirac notation familiar to physicists are :

$$|z\rangle := \hat{T}(z)|0\rangle \tag{1.1}$$

where :

$$|0\rangle(x) := (\pi\hbar)^{-n/4} \exp(-x^2/2\hbar)$$

is the (normalized) ground state of the Harmonic Oscillator

$$\hat{H}_0 = \frac{\hat{P}^2 + \hat{Q}^2}{2}$$

Let $\hat{H}$ be the Weyl quantization of a classical symbol, possibly depending on time $H(z,t)$ which satisfies the following assumption :

$$\exists m, M, K > 0 : \quad (1+z^2)^{-M/2} |\partial_z^\gamma H(z,t)| \leq K \quad \forall |\gamma| \geq m \tag{1.2}$$

uniformly for $(z,t) \in [-T,T] \times Z$

such that the classical and quantum evolutions respectively (for the classical symbol and its Weyl quantization resp.) exist for $t \in [-T,T]$.

Then it is well known that the stability around a trajectory of the classical flow $z \longrightarrow z_t$ is governed by the following **symplectic matrix** F_t obeying the linear equation :

$$\dot{F} = JM_tF \tag{1.3}$$

where M_t is the $2n \times 2n$ Hessian matrix of H at point z_t of the classical trajectory :

$$(M_t)_{j,k} := \left(\frac{\partial^2 H}{\partial z_j \partial z_k} \right)_{j,k} (z_t, t) \tag{1.4}$$

is symmetric real, and the initial datum is

$$F(0) \equiv \mathbb{1} \tag{1.5}$$

To this symplectic matrix can be associated a unitary operator in $\mathcal{H}$ of the **metaplectic group** (see tableau above) $\hat{R}(F_t)$. We denote by S_t the classical action along the classical flow $z \to z_t$:

$$S_t(z) := \int_0^t ds(\dot{q}_s.p_s - H(z_s, s)) \tag{1.6}$$

and we define :

$$\delta_s := S_t(z) - \frac{q_t.p_t - q.p}{2} \tag{1.7}$$

$$\Phi(z,t) := e^{i\delta_t/\hbar}\hat{T}(z_t)\hat{R}(F_t)|0\rangle \tag{1.8}$$

which is, up to the phase, a **squeezed state** located around the phase-space point z_t with a dispersion governed by the matrix F_t. We can prove the following estimate :

Theorem 1.1 *Let H be an Hamiltonian satisfying the assumptions (1.2) and the existence of classical and quantum flows for $t \in [-T, T]$. Then we have, uniformly for $(t, z) \in [-T, T] \times Z$:*

$$\|U_H(t,0)\varphi_z - \Phi(z,t)\| \leq C\mu(z,t)^P|t|\sqrt{\hbar}\theta(z,t)^3 \tag{1.9}$$

P being a constant only depending on M and m, and

$$\mu(z,t) := Sup_{0\leq s\leq t}(1 + |z_s|)$$

$$\theta(z,t) := Sup_{0\leq s\leq t}(trF_s^*F_s)^{1/2}$$

The estimate (1.9) contains the dependance in $t, \hbar, z$ of the semiclassical error term. One hopes that this error remains small when $\hbar \to 0$, provided that z belongs to some compact set of phase-space, and $|t|$ is not too large.

Typically

$$\theta(z,t) \simeq e^{t\lambda}$$

where λ is some Lyapunov exponent that expresses the "classical instability" near the classical trajectory. The RHS of equ. (3.36) is therefore $O(\hbar^{\epsilon/2})$ provided

$$|t| < \frac{1-\epsilon}{6\lambda}\log\hbar^{-1} \tag{1.10}$$

which is typically the Ehrenfest time, up to a factor 1/6 that is probably inessential.

For more details and prior references see [6].

2 What is a Trace Formula ?

Let $\mathcal{H} := L^2(\mathrm{R}^n)$ be the Hilbert space of Quantum States, and $\hat{H}$ be a selfadjoint quantum Hamiltonian acting on it. It genarates via Schrödinger Equation an unitary quantum evolution operator

$$U(t) := \exp(-it\hat{H}/\hbar) \tag{2.11}$$

We assume that the spectrum of $\hat{H}$ is pure point, namely :

$$sp(\hat{H}) = \{\lambda_k\}_{k \in \mathrm{N}} \tag{2.12}$$

Then for f sufficiently smooth and decreasing at infinity, $f(\hat{H})$ is a Trace Class Operator in $\mathcal{H}$. (it is enough for this that $\{f(\lambda_k)\}_{k \in \mathrm{N}} \in l^1$), and we have :

$$f(\hat{H}) := \sum_{k \in \mathrm{N}} f(\lambda_k) \tag{2.13}$$

The Trace Formula is simply :

$$tr f(\hat{H}) = something\ else \tag{2.14}$$

2.1 First Prototype : The Poisson summation Formula

Under suitable definition of the Fourier Transform $f \longrightarrow \tilde{f}$, we have :

$$\sum_{n=-\infty}^{+\infty} f(n) = \sum_{k=-\infty}^{+\infty} \tilde{f}(2k\pi) \tag{2.15}$$

which holds true for any $f \in \mathcal{S}(\mathrm{R}^n)$ (that implies of course that also $\tilde{f} \in \mathcal{S}(\mathrm{R}^n)$), and which is therefore perfectly symmetric between $f, \tilde{f}$.

Why do we mean that it is a Trace Formula ?

Consider the quantum operator in dimension 1 : $\hat{P} = -i\frac{d}{dx}$ acting on $L^2([0, 2\pi])$, with periodic boundary conditions $u(0) = u(2\pi)$. It is an unbounded operator, whose spectrum if purely discrete :

$$sp(\hat{P}) = \mathrm{Z}$$

Therefore the LHS of equ. (4.1) is nothing but $tr f(\hat{P})$.

What does the RHS represents physically ?

Imagine a classical Hamiltonian $H(q, p) := p$, where $q \in [0, 2\pi]$. ($\hat{P}$ is actually the Weyl quantization (for $\hbar = 1$) of H in $L^2([0, 2\pi])$ with Periodic Boundary conditions).

The associated Hamilton's equations are

$$\dot{q} = 1 \ , \ \dot{p} = 0$$

anf thus : $q = t \qquad (mod\ 2\pi)$

The classical trajectories are thus all closed ie periodic in phase space, and are **k-repetitions** of the primitive orbit of period $2\pi, \qquad \forall k \in \mathbf{Z}$. This means that the periods of the classical flow are of the form $2k\pi, \quad k \in \mathbf{Z}$.

The summation Poisson Formula thus expresses that the **trace of a function of a quantum Hamiltonian** of a very peculiar form is **the sum on the periodic orbits of the corresponding classical flow** of the Fourier Transform of that function taken at the periods of the classical flow.

2.2 Second Prototype : The Harmonic Oscillator in dimension 1

$$\hat{H}_0 := \frac{\hat{P}^2 + \hat{Q}^2}{2} \tag{2.16}$$

acting in $L^2(\mathrm{R})$ has spectrum $n + \frac{1}{2}$ (here again we let $\hbar = 1$), where $n \in \mathrm{N}$

Take $f \in \mathcal{S}([0, +\infty])$. Then obviously

$$tr f(\hat{H}_0) = \sum_{n=0}^{\infty} f(n + \frac{1}{2}) \tag{2.17}$$

Replace f by $\hat{T}(q, 0)f = f(. + q)$ in equ. (5.1). It becomes

$$\sum_{n \in \mathbb{Z}} f(n + q) = \sum_{k \in \mathbb{Z}} e^{2i\pi kq} \tilde{f}(2k\pi)$$

Thus taking $q = 1/2 \qquad e^{ik\pi} = (-1)^k$ which yields :

$$\sum_{n=0}^{\infty} f(n + \frac{1}{2}) = \sum_{k \in \mathbb{Z}} (-1)^k \tilde{f}(2k\pi) \tag{2.18}$$

Since the classical trajectories of the classical Harmonic Oscillator are of the form

$$q(t) = A sin(t + \alpha)$$

every orbit is therefore periodic, with a period which is a k-repetition of the primitive orbit of period 2π. The periods of the closed orbits of the classical flow are thus $\{2k\pi\}_{k \in \mathbb{Z}}$.

We see here a factor $(-1)^k \equiv e^{(2k)i\pi/2}$ which is here the first manifestation of a “Maslov Index” $2k$.

Here again, equ. (2.18) expresses that the trace of the function of a Quantum Hamiltonian can be written as a sum over the periodic orbits of the corresponding classical flow of the Fourier Transform of that function, taken at the periods of the classical flow, **up to some factor of the form $e^{\sigma_k i\pi/2}$ where σ_k is the Maslov index of the orbit**.

The important fact to notice is that “someting else” in the RHS of (2.4) is a sum over the periodic orbits of the classical flow, and that the miracle obtained above in the two Prototypes has a Prolongation in the semiclassical limit, as we shall see in the last Section.

3 Physical Motivations

Consider as an illustration the case of billiards in R^2 which are bounded domains $\Omega \in \mathrm{R}^2$ with a boundary denoted $\partial\Omega$ which is piecewise regular. Then two a priori not connected sets of problems can be addressed :

-on the Classical Side consider a point particle moving inside Ω with constant velocity, and specular reflections on the boundary $\partial\Omega$. We interest ourselves to the “spectrum” of lengths of periodic orbits inside the billiard. How are they distributed ?

-on the other hand the equivalent of a Quantum Problem is the study of the Dirichlet Laplacian in Ω. What is its spectrum and how is it distributed for large energies ?

Is there a link between these two Problems ? The answer is YES, semiclassically (that means asymptotically in the quantum spectrum). It somehow provides an answer of the famous V. Kac Question :

CAN WE HEAR THE SHAPE OF A DRUM ?

or of a paraphrased problem raised by C.A. Pillet :

CAN WE SEE THE SOUND OF A DRUM ?

The energy level density (defined in a distributional sense on suitable test functions) is the following :

$$d(E) := \sum_{k \in \mathrm{N}} \delta(E - \lambda_k) \tag{3.19}$$

Coming back to the traditional Schrödinger Hamiltonian, given E we can perform an average of $d(E)$ in a small neighborhood, which leads to the so-called "mean level density" $\bar{d}(E)$, and the first question to be addressed is that of finding a semiclassical approximation of it.
According to H. Weyl, we get :

$$\int \bar{d}(E) \simeq \frac{vol(energy\ shell\ \Sigma_E)}{h^n} \tag{3.20}$$

where as usual :

$$h := 2\pi\hbar \to 0 \tag{3.21}$$

and where the energy shell is :

$$\Sigma_E := \{z : \ H(z) = E\}$$

where H is the classical symbol of $\hat{H}$.

The physical intuition for it is that the LHS of (3.20) "counts" the average number of states at energy E, and that **one** quantum state occupies a volume of phase-space of size h^n

The next section to be raised is the nature of the quantum **fluctuations** of $d(E)$ around $\bar{d}(E)$. These appear to be different according to whether the classical dynamics generated by H is *regular, (integrable)*, or *chaotic*.

-in the *integrable* case, trace formulae can be obtained and the semiclassical behavior of $d(E) - \bar{d}(E)$ can be expanded as a "sum" over the invariant tori of the classical flow, as obtained heuristically by Berry-Tabor ([2]), and rigorously by Colin de Verdière ([4]) in the framework of compact manifolds.

-in the *chaotic* case as a sum over the unstable periodic of the classical flow, as suggested by Balian-Bloch ([1]), and Gutzwiller ([8]).

Notice that in the two last works cited, the proof is heuristic, the sum over the periodic orbits is **divergent**, and the correction terms in $\hbar$ are omitted. Rigorous proofs have been established and are due to Chazarain [3], Duistermaat-Guillemin [7], Paul-Uribe [10], Meinrenken [9], and Combescure-Ralston-Robert [5]. All these proofs, as an assumption, take the Gutzwiller Hypothesis that the unstable Periodic Orbits are **nondegenerate**, or a weaker assumption of "clean flow" , and furthermore **violate the beautiful classical/quantum duality** of the exact Trace Formulae, in that the test functions φ considered are assumed to have compact support in Fourier variable, which automatically truncates the sum over periodic orbits to those for which the period is in the support of $\tilde{\varphi}$.

4 Gutzwiller Trace Formula (Rigorous Proof)

The proof we want to present here is the simplest one which makes use of semiclassical estimates of the evolution of coherent states, as presented in Section 1. (Theorem 1.1). The main mathematical trick is the following :

$$tr\hat{A} = h^{-n} \int_Z dz \langle z|\hat{A}|z\rangle \tag{4.22}$$

for any **trace class operator** $\hat{A}$, and thus the following :

$$tr\varphi\left(\frac{\hat{H}-E}{\hbar}\right) = tr\left(\int dt e^{it(E-\hat{H})/\hbar}\tilde{\varphi}(t)\right)$$

$$= h^{-n}\int dt e^{itE/\hbar}\tilde{\varphi}(t)\int_Z dz\langle z|e^{-it\hat{H}/\hbar}|z\rangle$$

We shall now make precise our assumptions on H :

Assumptions

(H1) $H(\hbar, z) \asymp \sum_{j=0}^{\infty} \hbar^j H_j(z) \qquad H_j : Z \mapsto \mathrm{R} \in \mathcal{C}^\infty(Z)$

(H2) H_0 bounded from below and

$$0 \le H_0(z) + \gamma_0 \le C(H_0(z') + \gamma_0)(1 + |z - z'|)^M \quad \forall z, z' \in Z$$

(H3) $\forall j \in \mathrm{N}\ \forall \gamma \in \mathrm{N}^{2n} \quad |\partial_z^\gamma H_j(z)| \le C(H_0(z) + \gamma_0)$

(H4) $|\partial_z^\gamma (H(\hbar, z) - \sum_0^N \hbar^j H_j(z))| \le C(N, \gamma)\hbar^{N+1} \quad \forall \hbar \in (0, 1)$ uniformly for $z \in Z$

(H5) Let $I_{cl} :=]\lambda_-, \lambda_+[$ be an interval of classical energy, then $H_0^{-1}(I_{cl})$ is bounded in R^{2n} (the energy surfaces for $E \in I_{cl}$ are all compact)

(H6) E is a noncritical value for H_0 namely $H_0(z) = E \Rightarrow \nabla_z H_0 \neq 0$

We can prove the following result :

Theorem 4.1 *Let H satisfy (H1)-(H6), and $\hat{H}$ its Weyl quantization. Consider the classical flow $\phi_{H_0}^t$ of H_0 on $\Sigma_E : \{H_0(z) = E\}$, and denote by γ the periodic orbits of this flow. We assume in addition (Gutzwiller Hypothesis) that the Poincaré map*

P_γ doesn't have 1 as eigenvalue, namely that the orbits γ are **nondegenerate**. *Then for any $\varphi \in \mathcal{S}$: $\tilde{\varphi} \in \mathcal{C}_0^\infty$, we have, asymptotically as $\hbar \to 0$:*

$$tr\varphi\left(\frac{\hat{H}-E}{\hbar}\right) \asymp h^{-n}\left(\tilde{\varphi}(0)|\Sigma_E|\hbar + \sum_{j\geq 2}\hbar^j c_{0,j}(\tilde{\varphi})\right) \tag{4.23}$$

$$+\sum_\gamma \frac{e^{iS_\gamma/\hbar} + i\sigma_\gamma\pi/2}{|\det(\mathbb{1}-P_\gamma)^{1/2}|}\left(\tilde{\varphi}(T_\gamma)\frac{T_\gamma^*}{2\pi}e^{-i\int_\gamma H_1} + \sum_{j\geq 1}\hbar^j c_{\gamma,j}(\tilde{\varphi})\right)$$

where :
γ^* *is the primitive orbit corresponding to* γ
T_γ *(resp. T_γ^*) is the period of γ (resp. γ^*)*
σ_γ *is the Maslov index of* γ
S_γ *is the classical action along* γ
P_γ *is the Poincaré map of* γ
$c_{0,j}$ *are distributions supported in* $\{0\}$
$c_{\gamma,j}$ *are distributions supported in* $\{T_\gamma\}$

Note that the duality Quantum/Classical is violated by the condition that $\tilde{\varphi}$ is of compact support.
The First line of (5.7) corresponds to the "regular part" in $\hbar$, and we recognize the dominant Weyl term (with corrections in $\hbar$ that Gutzwiller had "omitted", or neglected...)
The Second line corresponds to the "oscillating part" in $\hbar$, which is, as expected, a sum over the periodic orbits of the classical flow (here truncated since $\tilde{\varphi}(T_\gamma) = 0$ for γ large).

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