Contemporary Mathematics

Trace Formulae

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Abstract. Rigorous versions of the Gutzwiller trace formula are discussed. Although the proofs are only sketched, the mathematical *raison d'être* of the formula is discussed in detail.

Contents

Introduction

The purpose of these notes is to discuss the Duistermaat-Guillemin trace formula and the semi-classical trace formula (the former just by an example). A higher goal is to introduce the reader to some ideas of semi-classical analysis, and to illustrate the use of its basic tools: Fourier analysis and the method of stationary phase. I do not intend to give complete proofs of the trace formulae, but I do give precise statements and discuss the main ideas involved in the proofs.

The contents of the notes are as follows. After discussing some generalities in Section 1.1, I derive the Duistermaat-Guillemin trace formula for a torus, $\mathbb{R}^n/\Gamma$. This follows simply from the Poisson summation formula and the method of stationary phase. Section 2 is devoted to the semi-classical trace formula. Discussion of the basic tools is relegated to three appendices: (A) on the Fourier transform, (B) on the method of stationary phase and (C) on the Hamilton-Jacobi equation.

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1. Some classical trace formulae

1.1. Generalities on trace formulae. Let $\mathcal{H}$ be a Hilbert space and Q a bounded operator on $\mathcal{H}$. We will assume that there exists an orthonormal basis $\{e_j\}$ of $\mathcal{H}$ such that

$$Q(e_j) = \nu_j\, e_j, \qquad \nu_j \in \mathbb{C}.$$

Definition 1.1. [1] Such an operator is said to be of trace-class iff the series $\sum_j \nu_j$ is absolutely convergent. In this case we define

$$\mathrm{Tr}(Q) := \sum_j \nu_j.$$

Suppose that $\mathcal{H} = L^2(M, d\mu)$ so that the e_j are functions on M. Then the Schwartz kernel of Q is by definition the following function on $M \times M$:

$$K(x,y) = \sum_j \nu_j\, e_j(x)\, \overline{e_j(y)} \tag{1.1}$$

(let's assume that the series is converges absolutely and uniformly), and it has the virtue that $\forall f \in \mathcal{H}$

$$Q(f)(x) = \int_M K(x,y)\, f(y)\, d\mu(y). \tag{1.2}$$

The following observation is perhaps the simplest trace formula:

$$\mathrm{Tr}(Q) = \int_M K(x,x)\, d\mu(x). \tag{1.3}$$

This follows easily from (1.1).

The most important operators with discrete spectrum arising in geometry and physics (e.g. the Laplace-Beltrami, Schrödinger and Dirac operators) are definitely *not* trace class. Suitable functions of them, however, are trace class. Specifically, let P be an unbounded operator on $\mathcal{H}$, and assume that there exists an orthonormal basis $\{e_j\}$ of $\mathcal{H}$ such that

$$P(e_j) = \lambda_j\, e_j$$

where we now assume the eigenvalues $\{\lambda_j\}$ to be real and accumulating only at $\pm\infty$. Let φ be a function on the real line and define the operator

$$Q_\varphi := \varphi(P),$$

that is, Q_φ is defined by the property:

$$\forall j \qquad Q_\varphi(e_j) = \varphi(\lambda_j)\, e_j.$$

It is clear that if φ decays sufficiently fast at $\pm\infty$ then Q_φ is of trace class, and therefore for all such φ's

$$\sum_j \varphi(\lambda_j) = \int_M K_\varphi(x,x)\, d\mu(x), \tag{1.4}$$

[1] The general definition is as follows: a general bounded Q is of trace class iff for some orthonormal basis $\{e_j\}$ one has: $\sum_j < |Q|e_j, e_j >< \infty$, where $|Q| = \sqrt{QQ^*}$. Then $\mathrm{Tr}(Q) = \sum_j < Qe_j, e_j >$ is a finite number independent of the orthonormal basis; see [**18**] for details.

where K_φ is the Schwartz kernel of Q_φ. One usually regards φ as a *test function* (i.e. a variable), and then the formula (1.4) is a formula for the spectral measure of P.

With a few notable exceptions, there is no hope of being able to compute $\mathrm{Tr}(Q_\varphi)$ exactly. In all the trace formulae that we will discuss however, one computes (at least approximately) the kernel K_φ by writing:

$$Q_\varphi = \varphi(P) = \int e^{-itP}\, \check{\varphi}(t)\, dt, \tag{1.5}$$

where

$$\check{\varphi}(t) := \frac{1}{2\pi} \int e^{it\lambda}\, \varphi(\lambda)\, d\lambda$$

is the inverse Fourier transform of φ. Let's be more precise. Introduce the t-dependent operator

$$U(t) := e^{-itP}, \tag{1.6}$$

defined by the property:

$$\forall j \qquad U(t)\,(e_j) = e^{-it\lambda_j}\, e_j.$$

Then, by the Fourier inversion formula $\forall f \in \mathcal{H}$

$$\varphi(P)(f)(x) = \int U(t)(f)(x)\, \check{\varphi}(t)\, dt. \tag{1.7}$$

The Schwartz kernel of $U(t)$[2] is:

$$U(t,x,y) := \sum_j e^{-it\lambda_j}\, e_j(x)\, \overline{e_j(y)}. \tag{1.8}$$

The advantage of introducing $U(t)$ is that *it solves the following equation*:

$$\frac{1}{i}\frac{\partial}{\partial t} U(t) = -P\,(U(t)), \tag{1.9}$$

with the initial condition

$$U(t)|_{t=0} = I. \tag{1.10}$$

The idea behind the trace formula is: *to solve, at least approximately, the problem (1.9,1.10) and then to write:*

$$\sum_j \varphi(\lambda_j) = \int\!\!\int U(t,x,x)\, \check{\varphi}(t)\, dt\, d\mu(x). \tag{1.11}$$

(In the cases we are interested in this formula makes sense as an iterated integral.)

We will next study some classical cases when the program above can be worked out exactly. In each case we will specify a Hilbert space $\mathcal{H}$ and an operator P, and will compute the right-hand side of (1.11) to get a non-trivial formula.

[2]Strictly speaking this only exists in the sense of distribution theory

1.2. The Poisson summation formula. There are many proofs of this famous relation but here we present one in the spirit of §1.1. Let $T > 0$ and let

$$\mathcal{H} \;=\; L^2(S^1_T) \;=\; \{\, f : \mathbb{R} \to \mathbb{C};\ f \text{ is } T \text{ periodic and } \int_0^T |f(x)|^2\, dx < \infty \,\}.$$

Let also

$$P \;:=\; D_x \;:=\; \frac{1}{i}\,\frac{d}{dx}.$$

Then the orthonormal eigenfunctions and eigenvalues of P are

$$\forall j \in \mathbb{Z} \quad e_j(x) \;=\; \frac{1}{\sqrt{T}}\, e^{ij\omega x}\,, \qquad \lambda_j \;=\; j\omega \quad \text{where } \omega \;=\; \frac{2\pi}{T}. \tag{1.12}$$

In this case the operator $U(t) = e^{-itP}$ is the translation operator

$$U(t)(f)(x) \;=\; f(x-t), \tag{1.13}$$

since

$$\frac{\partial}{\partial t}\, f(x-t) \;=\; \frac{df}{dx}(x-t). \tag{1.14}$$

(The reader might recognize in $f(x-t)$ a solution to the one-dimensional wave equation, in fact (1.14) is a *square root* of the wave equation.) It follows from (1.7) that if φ decays rapidly at infinity,

$$\varphi(P)(f)(x) \;=\; \int_{-\infty}^{+\infty} f(x-t)\, \check{\varphi}(t)\, dt.$$

Departing slightly from the general scheme outlined in §1.1, we will now see that we can get from this expression a formula for the Schwartz kernel of $\varphi(P)$. First, split the integral along intervals of length T:

$$\int_{-\infty}^{+\infty} f(x-t)\, \check{\varphi}(t)\, dt \;=\; \sum_{k=-\infty}^{+\infty} \int_{kT}^{(k+1)T} f(x-t)\, \check{\varphi}(t)\, dt$$

In the k-th summand make the change of variables: $s = t - kT$ and recall that f is T-periodic to obtain that the above expression equals

$$\sum_{k=-\infty}^{+\infty} \int_0^T f(x-t)\, \check{\varphi}(s+kT)\, ds \;=\; \int_0^T f(x-s)\, \tilde{\varphi}(s)\, ds,$$

where

$$\tilde{\varphi}(s) \;:=\; \sum_k \check{\varphi}(s+kT).$$

(These manipulations are valid if $\check{\varphi}$ decays sufficiently fast at infinity.) It is obvious that $\tilde{\varphi}$ is T-periodic. Letting $x = s - t$, we finally obtain

$$\varphi(P)(f)(x) \;=\; \int_0^T f(t)\, \tilde{\varphi}(x-t)\, dt,$$

from where it follows that the kernel of $\varphi(P)$ is:

$$K_\varphi(x,y) \;=\; \tilde{\varphi}(x-y).$$

Applying (1.4) and taking into account (1.12) we finally obtain:

$$\sum_{j=-\infty}^{+\infty} \varphi(j\omega) \;=\; \int_0^T \check{\varphi}(0)\,dx \;=\; T \sum_{k=-\infty}^{+\infty} \check{\varphi}(kT). \tag{1.15}$$

This is the Poisson summation formula:

THEOREM 1.2. *For all $T > 0$ and for all Schwartz functions φ on $\mathbb{R}$*

$$\sum_{j=-\infty}^{+\infty} \varphi(j\omega) \;=\; T \sum_{k=-\infty}^{+\infty} \check{\varphi}(kT)$$

where $\omega = 2\pi/T$ and $\check{\varphi}$ is the inverse Fourier transform of φ.

For our purposes, this is to be understood as follows. The left-hand side is the trace of $\varphi(D_x)$ (acting on $L^2(S^1_T)$); ω is the fundamental frequency of the circle. It is therefore an analytic quantity. The right-hand side involves the length of the circle, T, which is a *geometric* quantity. This is a typical feature of trace formulae. The relationship involves an integral transform of the test function. For the asymptotic (or semi-classical) trace formula this integral transform will always be the Fourier transform.

1.3. The n-dimensional torus. In this section we generalize the above considerations from the circle to the n-dimensional torus. There is a standard way of generalizing the Poisson summation formula to n dimensions, involving Schwartz functions of n variables (see for example [**9**]). What we want to do here however is to present a generalization that will hopefully motivate the semi-classical trace formula of §2.

Let $\Gamma \subset \mathbb{R}^n$ be a lattice, and $M := \mathbb{R}^n/\Gamma$ be an n-torus. We let $\mathcal{F}$ be a fundamental domain for Γ, and we identify $\mathcal{H} := L^2(M)$ with the space of Γ-periodic functions on $\mathbb{R}^n$ with the norm

$$\| f \|^2 \;=\; \int_{\mathcal{F}} |f(x)|^2\,dx,$$

where dx is Lebesgue measure on $\mathbb{R}^n$. (By Γ-periodicity we mean: $\forall x \in \mathbb{R}^n,\ \gamma \in \Gamma \quad f(x+\gamma) = f(x)$.) The space of Γ-periodic functions is preserved by the Laplacian,

$$\Delta = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}.$$

The eigenfunctions of Δ on $\mathcal{H}$ are the exponentials in that space. Thus we must introduce the dual lattice,

$$\Gamma^* \;:=\; \{\, k \in \mathbb{R}^n \;;\; \forall \gamma \in \Gamma \quad k\cdot\gamma \in 2\pi\mathbb{Z} \,\}.$$

The eigenfunctions of Δ on $\mathcal{H}$ are the functions:

$$\forall k \in \Gamma^* \qquad e_k(x) \;:=\; e^{ik\cdot x},$$

the corresponding eigenvalue being $-\|k\|^2$.

The operator that we will consider here is the positive square root of $-\Delta$ acting on $\mathcal{H}$:

$$P \;:=\; \sqrt{-\Delta}\,|_{\mathcal{H}}.$$

Therefore the eigenfunctions of P are again the e_k, $k \in \Gamma^*$ the eigenvalue being now $\|k\|$, the length of k. The reason for introducing the square root is that then the equation satisfied by $U(t) = e^{-itP}$ is the *wave equation*: Differentiating $U(t)$ twice with respect to t we get:

$$\frac{\partial^2}{\partial t^2} U(t) \;=\; \Delta(U(t)).$$

According to the general scheme outlined in §1.1, the trace formula for P is obtained by computing the right-hand side of the relation

$$\sum_{k\in\Gamma^*} \varphi(\|k\|) \;=\; \int\int_{\mathcal{F}} U(t,x,x)\,\check{\varphi}(t)\,dx\,dt.$$

Let $\tilde{U}(t,x,y)$ be the Schwartz kernel of the operator $e^{-it\sqrt{-\Delta}}$ on $L^2(\mathbb{R}^n)$. On the one hand, by the properties of the Fourier transform we see that

$$\tilde{U}(t)(f)(x) \;=\; \frac{1}{(2\pi)^n}\int e^{i[x\cdot\xi - t\|\xi\|]}\,\hat{f}(\xi)\,d\xi, \tag{1.16}$$

which we write (formally, if the reader wishes) as:

$$\tilde{U}(t,x,y) \;=\; \frac{1}{(2\pi)^n}\int e^{i[(x-y)\cdot\xi - t\|\xi\|]}\,d\xi. \tag{1.17}$$

On the other it is trivial to check (from general considerations) that

$$U(t,x,y) \;=\; \sum_{\gamma\in\Gamma} \tilde{U}(t, x+\gamma, y). \tag{1.18}$$

Putting these things together we obtain:

$$\begin{aligned}\sum_{k\in\Gamma^*}\varphi(\|k\|) \;&=\; \frac{1}{(2\pi)^n}\sum_{\gamma\in\Gamma}\int\int\int e^{i[(x+\gamma-x)\cdot\xi - t\|\xi\|]}\,\check{\varphi}(t)\,dx\,dt\,d\xi \\ &=\; \frac{|\mathcal{F}|}{(2\pi)^n}\sum_{\gamma\in\Gamma}\int e^{i\gamma\cdot\xi}\,\varphi(\|\xi\|)\,d\xi. \end{aligned}\tag{1.19}$$

where $|\mathcal{F}|$ denotes the volume of $\mathcal{F}$ (i.e. the volume of the torus, M). It is clear that the expression

$$\frac{1}{(2\pi)^n}\int e^{i\gamma\cdot\xi}\,\varphi(\|\xi\|)\,d\xi,$$

ostensibly a function of γ, is really just a function of $\|\gamma\|$. (We can compensate a rotation of γ by a change of variables that also rotates ξ.) Passing to polar coordinates in $\mathbb{R}^n$ (i.e. letting $\xi = r\eta$ with $\|\eta\| = 1$), we can rewrite the above as

$$\frac{1}{(2\pi)^n}\int_0^\infty\int_{S^{n-1}} e^{ir\gamma\cdot\eta}\,\varphi(r)\,r^{n-1}\,d_{S^{n-1}}(\eta)\,dr$$

where $d_{S^{n-1}}$ denotes the standard measure on the $(n-1)$-dimensional sphere, S^{n-1}. We can summarize these results as follows:

THEOREM 1.3. *For every Schwartz function φ let*

$$\tilde{\varphi}(s) \;:=\; \frac{1}{(2\pi)^n}\int_0^\infty\int_{S^{n-1}} e^{isr\eta_1}\,\varphi(r)\,r^{n-1}\,d_{S^{n-1}}(\eta)\,dr. \tag{1.20}$$

Then one has:

$$\sum_{k\in\Gamma^*} \varphi(\|k\|) \;=\; |\mathcal{F}| \sum_{\gamma\in\Gamma} \tilde{\varphi}(\|\gamma\|). \tag{1.21}$$

This is the *exact* trace formula for the Laplacian on the torus $\mathbb{R}^n/\Gamma$; it involves the unusual integral transform $\varphi \mapsto \tilde{\varphi}$. *Notice that* $\|\gamma\|$ *is precisely the length of the geodesics on the torus in the homology class of* γ*, while* $\{\|k\|\,;\,k\in\Gamma^*\}$ *is the spectrum of* P. Once again the interpretation of (1.21) is: The left-hand side is spectral, the right-hand side geometric.

In the particular case when the test function is the Gaussian $\varphi(w) \;=\; e^{-w^2t}$ where here t is regarded as a parameter, then one can compute $\tilde{\varphi}(u) \;=\; \frac{1}{(4\pi t)^{n/2}}\, e^{-u^2/4t}$, and we obtain the celebrated Jacobi identity for the Dirichlet series associated with Γ:

$$\sum_{k\in\Gamma^*} e^{-\|k\|^2 t} \;=\; \frac{|\mathcal{F}|}{(4\pi t)^{n/2}} \sum_{\gamma\in\Gamma} e^{-\|\gamma\|^2/4t}. \tag{1.22}$$

One can interpret this as a formula for the trace of $e^{-t\Delta}$ (the fundamental solution of the heat equation on the torus) acting on $\mathcal{H}$.

I have pointed out that in the asymptotic trace formulae to be discussed in the next chapter the integral transform of the test function that arises is always the Fourier transform. Let us see how this comes about, in the present setting. In the asymptotic trace formula for the square root of the Laplacian due to Duistermaat and Guillemin, [**8**], one looks at large eigenvalues only. This is achieved by translating the test function φ by an amount μ and letting $\mu\to\infty$. Specifically, in the present case one should consider the asymptotic behavior of

$$\sum_{k\in\Gamma^*} \varphi(\|k\|-\mu) \quad \text{as } \mu\to\infty. \tag{1.23}$$

If we let, $\forall\ \mu$

$$\varphi_\mu(\lambda) \;:=\; \varphi(\lambda-\mu)$$

then we can apply Theorem 1.3 to φ_μ and obtain an exact formula involving $\widetilde{\varphi_\mu}$:

$$\widetilde{\varphi_\mu}(s) \;=\; \frac{1}{(2\pi)^n} \int_0^\infty \int_{S^{n-1}} e^{isr\eta_1}\, \varphi(r-\mu)\, r^{n-1}\, d_{S^{n-1}}(\eta)\, dr. \tag{1.24}$$

Let us raise the problem of estimating this quantity as $\mu\to\infty$, with s fixed (think of s as the length of a closed geodesic). We must distinguish two cases:

$\underline{s=0}$. (This is what what one calls “the Weyl term”.) One can compute directly:

$$\widetilde{\varphi_\mu}(0) \;=\; \frac{\mathrm{Vol}(S^{n-1})}{(2\pi)^n} \int_0^\infty \varphi(r-\mu)\, r^{n-1}\, dr.$$

Making the change of variables $u := r-\mu$, one gets

$$\widetilde{\varphi_\mu}(0) \;=\; \frac{\mathrm{Vol}(S^{n-1})}{(2\pi)^n} \int_{-\mu}^\infty \varphi(u)\, (u+\mu)^{n-1}\, du.$$

Expanding the binomial and noting that $\int \varphi(u)u^j\,du$ is, up to a multiplicative constant, equal to $\check{\varphi}^{(j)}(0)$, we can write the above as:

$$\widetilde{\varphi_\mu}(0) \sim \mu^{n-1}\,\mathrm{Vol}(S^{n-1})\,\check{\varphi}(0) + \sum_{j=1}^{n-1} \alpha_j(\check{\varphi})(0)\,\mu^{n-1-j} \tag{1.25}$$

where α_j is a differential operator of order j. Therefore this term is of order $O(\mu^{n-1})$ and, up to universal constants, the leading coefficient is $\int \varphi(u)du$.

$\underline{s>0}$. Make once again in (1.24) the change of variables $u := r-\mu$. Then the leading term in μ is

$$\widetilde{\varphi_\mu}(s) \sim \frac{1}{(2\pi)^n}\,\mu^{n-1}\int_{-\mu}^{\infty}\int_{S^{n-1}} e^{is(\mu+u)\eta_1}\,\varphi(u)\,d_{S^{n-1}}(\eta)\,du; \tag{1.26}$$

the lower order terms simply have an extra factor of u^j in the integrand (and can be estimated in a similar way as the leading term). We can write the leading term (1.26) as

$$\frac{1}{(2\pi)^n}\,\mu^{n-1}\int_{S^{n-1}} e^{is\mu\eta_1}\left(\int_{-\mu}^{\infty} e^{isu\eta_1}\,\varphi(u)\,du\right)d_{S^{n-1}}(\eta).$$

The term in parenthesis, combined with the constant in front of the expression, converges to $\check{\varphi}(s\eta_1)$. Now we appeal to the method of stationary phase. The function on the sphere $\eta \mapsto s\eta_1$ clearly has two critical points, a maximum at $\eta = (1,0,\dots 0)$ and a minimum at $\eta = (-1,0,\dots,0)$. Therefore the method of stationary phase yields:

$$\widetilde{\varphi_\mu}(s) \sim (2\pi)^{\frac{n-1}{2}}\,\mu^{\frac{n-1}{2}}\left(e^{i\mu s}\sum_{j=0}^{\infty} c_j^+(\check{\varphi})(s) + e^{-i\mu s}\sum_{j=0}^{\infty} c_j^-(\check{\varphi})(-s)\right), \tag{1.27}$$

where the $c_j^\pm$ are differential operators; in particular

$$c_0^\pm(\check{\varphi}) = e^{\pm i(1-n)\pi/4}\,\check{\varphi}. \tag{1.28}$$

Combining these estimates we get the following result:

THEOREM 1.4. *For each test function φ such that $\check{\varphi} \in C_0^\infty(\mathbb{R})$ one has the following asymptotic expansion as $\mu \to \infty$:*

$$\sum_{k\in\Gamma^*} \varphi(\|k\|-\mu) \sim \mu^{n-1}\;Vol(S^{n-1})\,|\mathcal{F}|\,\check{\varphi}(0) + \sum_{j=1}^{n-1}\alpha_j(\check{\varphi})(0)\,\mu^{n-1-j} + \tag{1.29}$$

$$+\,|\mathcal{F}|\,(2\pi)^{\frac{n-1}{2}}\,\mu^{\frac{n-1}{2}}\sum_{\gamma\in\Gamma\setminus\{0\}}\left(e^{i\mu\|\gamma\|}\sum_{j=0}^{\infty} c_j^+(\check{\varphi})(\|\gamma\|)\,\mu^{-j} + e^{-i\mu\|\gamma\|}\sum_{j=0}^{\infty} c_j^-(\check{\varphi})(-\|\gamma\|)\,\mu^{-j}\right),$$

where (1.28) holds.

This is precisely a particular case of the Duistermaat-Guillemin trace formula, [**8**], for $\sqrt{-\Delta}$ on $\mathbb{R}^n/\Gamma$. The semi-classical trace formula is an identity of the same type. Let us make a series of remarks that are typical of these formulae.

Remarks:

1. The leading term of the expansion is the leading Weyl term, $\mu^{n-1}\mathrm{Vol}(S^{n-1})|\mathcal{F}|\check{\varphi}(0)$. The Weyl term

$$\mu^{n-1}\,\mathrm{Vol}(S^{n-1})\,|\mathcal{F}|\,\check{\varphi}(0)\,+\,\sum_{j=1}^{n-1}\alpha_j(\check{\varphi})(0)\,\mu^{n-1-j} \tag{1.30}$$

in this case is a polynomial in μ. For the general semi-classical trace formula it is an asymptotic series in decreasing powers of μ. Notice that (1.30) vanishes if $\check{\varphi}$ is supported away from zero. This serves as a definition of the Weyl term in the general case.

2. Since the $c_j^{\pm}$ are differential operators, under the assumption on $\check{\varphi}$ the sum over $\gamma \in \Gamma \setminus \{0\}$ is finite. *This sum is to be understood as a sum over the periodic geodesics on the torus.* Notice the exponential factors that make the sum oscillatory as $\mu \to \infty$.

3. If we pick $\check{\varphi}$ supported away from zero then as we have said the Weyl terms vanish and therefore the leading term in the expansion is

$$|\mathcal{F}|\,(2\pi)^{\frac{n-1}{2}}\,\mu^{\frac{n-1}{2}}\sum_{\gamma\in\Gamma\setminus\{0\}}\left(e^{i\mu\|\gamma\|}\check{\varphi}(\|\gamma\|)\,+\,e^{-i\mu\|\gamma\|}\check{\varphi}(-\|\gamma\|)\right), \tag{1.31}$$

i.e. the sum over periodic geodesics provides the leading term. (If $n = 2$ (1.31) is the sub-principal term in the expansion, regardless of the support of $\check{\varphi}$.)

4. If φ is real-valued then $\check{\varphi}(-s) = \overline{\check{\varphi}(s)}$ and then the leading contribution of the sum over periodic geodesics can be written as

$$2|\mathcal{F}|\,(2\pi)^{\frac{n-1}{2}}\,\mu^{\frac{n-1}{2}}\sum_{\gamma\in\Gamma\setminus\{0\}}\Re(e^{i[(1-n)\pi/4+\mu\|\gamma\|]}\,\check{\varphi}(\|\gamma\|)).$$

If φ is real-valued and even then $\check{\varphi}$ is real-valued and the above becomes

$$2|\mathcal{F}|\,(2\pi)^{\frac{n-1}{2}}\,\mu^{\frac{n-1}{2}}\sum_{\gamma\in\Gamma\setminus\{0\}}\cos\left(\mu\|\gamma\|+(1-n)\frac{\pi}{4}\right)\check{\varphi}(\|\gamma\|).$$

2. The semi-classical trace formula

The trace formula of §1 was for $P = \sqrt{-\Delta}$ on the torus, and the equation solved by e^{-itP} was the wave equation. Theorem 1.4 is an asymptotic result where one looks at the large eigenvalues of P. As mentioned, this sort of result holds under very general conditions (for e.g. the Laplacian on a generic compact Riemannian manifold); it's the Duistermaat-Guillemin trace formula, [**8**].

In this chapter we will discuss another trace formula, where the relevant operator is the Schrödinger operator,

$$P\,=\,P_\hbar\,=\,-\hbar^2\Delta+V \tag{2.1}$$

and the associated equation is the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi\,=\,P(\psi). \tag{2.2}$$

The asymptotic regime that we are interested in is as $\hbar \to 0$. This leads to the semi-classical trace formula (STF for short). The first to argue that a result of this kind ought to be true was Martin Gutzwiller, [**10**], and therefore the STF is also called the Gutzwiller trace formula. (Gutzwiller's formulation was in precisely the same spirit as the Theorem below, but his statement is different from ours and is unproven to-date. It appears that it does not always holds.)

The history of the rigorous STF is somewhat involved. First statements, involving the square roots of the eigenvalues, were first obtained in [**12**] and [**5**]. The statement presented below was first announced by T. Paul and A. Uribe in [**16**], with the details of the proof published in [**17**]. Independently, E. Meinrenken announced the same results in [**15**] (see also Dozias, [**6**]). For further details, see the overview paper by Bernard Helffer, [**13**]

For simplicity we will work on $\mathbb{R}^n$. We consider the operator (2.1), where Δ is the Laplacian on $\mathbb{R}^n$ and $V \in C^\infty(\mathbb{R}^n)$. Let us assume throughout that V tends to $+\infty$ at infinity. It is known that this implies that if $\hbar$ is small enough the spectrum of $P_\hbar$ on $L^2(\mathbb{R}^n)$ is discrete; there exists an orthonormal basis $\{\psi_{j,\hbar}\,;\, j = 1,\dots\}$ of $L^2(\mathbb{R}^n)$ of eigenfunctions of $P_\hbar$. Denote by $E_{j,\hbar}$ the associated eigenfunctions:

$$P_\hbar(\psi_{j,\hbar}) \;=\; E_{j,\hbar}\,\psi_{j,\hbar}. \tag{2.3}$$

The semi-classical trace formula is associated to the equation (2.2) in the sense that it "computes" (in fact simply estimates) the trace of

$$Q^\hbar_\varphi \;=\; \int e^{-i\hbar t P_\hbar}\,\check{\varphi}(t)\,dt. \tag{2.4}$$

(Notice that the exponential appearing on the right-hand side is the fundamental solution of (2.2).) A simple calculation will convince the reader that

$$\mathrm{Tr}(Q^\hbar_\varphi) \;=\; \sum_j \varphi\left(\frac{E_{j,\hbar}}{\hbar}\right). \tag{2.5}$$

This is the type of quantity that we'll estimate. If we keep in mind that φ is rapidly decreasing, we see that (2.5) examines the spectrum in a neighborhood of zero. If we want to examine the spectrum in a neighborhood of a given $E \in \mathbb{R}$, then we should generalize (2.5) to

$$\sum_j \varphi\left(\frac{E_{j,\hbar} - E}{\hbar}\right) \tag{2.6}$$

This is of course the same as shifting $P_\hbar$ by E. The semi-classical trace formula is an asymptotic expansion of (2.6), as $\hbar \to 0$, valid under certain fairly general conditions. To explain the terms appearing in the expansion, we must digress and explain several concepts from classical mechanics.

2.1. Classical mechanics. (See [**1**], [**2**] for general background.) The trajectories $x(t)$ of a classical particle on $\mathbb{R}^n$ under the influence of the force $\vec{F} = -\nabla V$ satisfy Newton's second law (we'll take the mass of the particle to be one),

$$\forall\, t \qquad \frac{d^2}{dt^2}x(t) \;=\; -\nabla V(x(t)).$$

As usual this second-order equation can be replaced by an equivalent first-order system:

$$\begin{cases} \frac{d}{dt}x(t) &=& p(t) \\ \frac{d}{dt}p(t) &=& -\nabla V(x(t)) \end{cases} \tag{2.7}$$

where the first equation is the definition of $p(t)$, the momentum of the trajectory at time t. More specifically, one introduces the space $\mathbb{R}^n \times \mathbb{R}^n$ of all possible positions and momenta, (x,p). This is called phase space. On it one can define the Hamiltonian (or total energy function)

$$H(x,p) = \frac{1}{2}\|p\|^2 + V(x) \tag{2.8}$$

and the associated Hamilton vector field

$$\Xi_{(x,p)} := \sum_{j=1}^{n} \frac{\partial H}{\partial p_j}\frac{\partial}{\partial x_j} - \frac{\partial H}{\partial x_j}\frac{\partial}{\partial p_j} = \sum_{j=1}^{n} p_j\,\frac{\partial}{\partial x_j} - \frac{\partial V}{\partial x_j}\,\frac{\partial}{\partial p_j}. \tag{2.9}$$

The flow of Ξ is called the Hamilton flow of H. The fundamental property of Ξ is that the equation satisfied by its integral curves is precisely the system (2.7). Therefore the projections onto position (that is x) space of the integral curves of Ξ are precisely the solutions to Newton's equation, and each integral curve is specified uniquely by an initial position and momentum.

We next review some concepts and results that appear in the statement of the semi-classical trace formula.

1. A basic property of the Hamilton flow is that energy is preserved: If $(x(t),p(t))$ is a solution of (2.7), then $H(x(t),p(t))$ is independent of t. In other words, the vector field Ξ is tangent to the family of hypersurfaces in $\mathbb{R}^{2n}$,

$$\Sigma_E := H^{-1}(E), \qquad E \in \mathbb{R} \tag{2.10}$$

These are called "energy surfaces". (Of course for some values of E Σ_E might not be smooth.)

2. Suppose that E is such that ∇H is not zero anywhere on Σ_E. Then Σ_E is smooth. We claim that it carries a natural measure, called the Liouville measure, that is preserved by the Hamilton flow.

3. Suppose that $\gamma(t) = (x(t),p(t))$ is a trajectory of Ξ. We call γ periodic of period $T \in \mathbb{R}$ iff $\gamma(t+T) = \gamma(t)$. (If this happens for some t it happens for all t.) If γ is periodic, its *primitive period* is the smallest $T > 0$ that is a period of γ.

4. Suppose that γ is periodic, T be a period and let E be its energy, so that $\gamma \subset \Sigma_E$. Let (x_0,p_0) be a point of γ. A *Poincaré section of* γ is a smooth $(n-2)$-dimensional surface S such that

$$(x_0,p_0) \in S \subset \Sigma_E \text{ and } \Xi_(x_0,p_0) \text{ is not tangent to } S.$$

Given a Poincaré section S, one can define a return map, $R : S \to S'$, where S' is a possibly smaller Poincaré section, by following the trajectories of Ξ emanating from points of S. Obviously $R(x_0,p_0) = (x_0,p_0)$, by the periodicity of γ. The *Poincaré map* of γ (associated to the period T) is by definition the differential of R at (x_0,p_0).

DEFINITION 2.1. The periodic trajectory γ is said to be non-degenerate iff the number 1 is not an eigenvalue of its Poincaré map.

Informally one can say that a periodic trajectory is non-degenerate if infinitesimally there are not any other periodic trajectories nearby with the same energy. It can be shown that non-degenerate periodic trajectories are isolated on the energy surface. On the other hand, if one lets the energy vary a non-degenerate γ belongs to a smooth family of periodic trajectories, indexed by the energy in some open interval.

2.2. The statement. The assumptions in the STF are on the Hamilton flow of H on the energy surface Σ_E where E has the same value as in (2.6). To begin with, we assume:

$$E \ \text{ is a regular value of } H\,, \tag{2.11}$$

so that Σ_E is a smooth $(2n-1)$-dimensional manifold. It is compact by the assumption that V tends to infinity at infinity. Physically, (2.11) says that there are no equilibria with energy E. Without this assumption, the asymptotics of (2.6) can include logarithmic terms in $\hbar$, and half-integral powers of $1/\hbar$; a first case of this situation was analyzed in [**4**]. Finally, we'll assume

$$\begin{gathered}\text{all periodic trajectories of the Hamilton flow of } H\\ \text{on } \Sigma_E \text{ are non-degenerate.}\end{gathered} \tag{2.12}$$

For a more general setting see [**17**].

Theorem 2.2. *Under the assumptions (2.11) and (2.12), for each test function φ such that $\check\varphi \in C_0^\infty(\mathbb{R})$ one has an asymptotic expansion of (2.6) as $\hbar \to 0$ of the form*

$$\sum_{j=1}^{\infty} \varphi\left(\frac{E_{j,\hbar}-E}{\hbar}\right) \sim \hbar^{1-n}\, LVol(\Sigma_E)\, \check\varphi(0) + \sum_{j=1}^{\infty} c_j(\check\varphi)(0)\, \hbar^{1-n+j} + \tag{2.13}$$

$$+\sum_\gamma e^{i\hbar^{-1}\int_\gamma p\,dx}\, e^{\pi i \mu_\gamma/4} \sum_{j=0}^{\infty} c_{\gamma,j}(\check\varphi)(T_\gamma)\, \hbar^j\,,$$

where:

1. *$LVol(\Sigma_E)$ is the Liouville measure of Σ_E.*
2. *The c_j and $c_{\gamma,j}$ are differential operators.*
3. *The sum $\sum_\gamma$ is over the periodic trajectories of the Hamilton flow of H and T_γ is the period of γ. This sum is finite.*
4. *μ_γ is an integer, the Maslov index of the trajectory γ.*
5. *The leading coefficient of the γ term is*

$$c_{\gamma,0}(\check\varphi)(T_\gamma) \;=\; \frac{T_\gamma^\sharp}{2\pi}\,\frac{1}{\sqrt{|\det(I-P_\gamma)|}}\,\check\varphi(T_\gamma), \tag{2.14}$$

where $T_\gamma^\sharp$ and P_γ are, respectively, the primitive period and the Poincaré map of γ.

Notice that the non-degeneracy assumption (2.12) ensures that $\det(I-P_\gamma) \neq 0$. Notice also that the contribution of the periodic trajectories is of order $O(1)$ in $\hbar$, whereas in Theorem 1.4 it was of order $O(\hbar^{(1-n)/2})$. This is because the assumption (2.12) implies that that the trajectories γ are isolated, whereas the geodesics on the torus come in n-dimensional families.

2.3. Sketch of the proof. Although the proof of Theorem 2.2 involves many technical details, it is possible to describe the gist of the argument using only the method of stationary phase and features of the Hamilton-Jacobi equation. This is what we will do now.

The basic idea (which has applications other than to the trace formula) is to construct an approximation to the Schwartz kernel of the propagator,

$$U(t,x,y) \;=\; \sum_j e^{-i\hbar^{-1}tE_{j,\hbar}}\,\psi_{j,\hbar}(x)\,\overline{\psi_{j,\hbar}(y)}, \tag{2.15}$$

fundamental solution to the Schrödinger equation. It should be clear that

$$\sum_{j=1}^{\infty}\varphi\left(\frac{E_{j,\hbar}-E}{\hbar}\right) \;=\; \int e^{it\hbar^{-1}E}\,U(t,x,x)\,\check{\varphi}(t)\,dt\,dx \tag{2.16}$$

and therefore estimates on the sums (2.6) would follow from having a sufficiently good approximation to U, valid for small $\hbar$.

The ansatz of the approximation to U is as follows:

$$U(t,x,y) \;=\; \int e^{i\hbar^{-1}[S(t,x,p)-y\cdot p]}\,a(t,x,y,p,\hbar)\,dp, \tag{2.17}$$

where S and a are to be determined. One postulates that a should have an asymptotic expansion of the form

$$a(t,x,y,p,\hbar) \sim \sum_{j=0}^{\infty} a_j(t,x,y,p)\,\hbar^j. \tag{2.18}$$

The reader might wonder where this ansatz comes from. Perhaps a sufficient answer is that (2.17) is a reasonable generalization of the form of the fundamental solution to the wave equation on $\mathbb{R}^n$, (1.17). In fact there is a long history of looking for approximate solutions to the Schrödinger equation of the form

$$\psi(t,x) \;=\; e^{i\hbar^{-1}S(t,x)}$$

called WKB solutions. One can view (2.17) as a superposition of WKB solutions, weighted by the amplitude a. The idea of looking for WKB solutions itself comes from geometrical optics in the 19th century.

Let us formally compute with (2.17). Let us write down the equation that U satisfies, namely

$$(-\hbar^2\Delta_x + V(x))\,U(t,x,y) \;=\; i\frac{\partial}{\partial t}\,U(t,x,y), \tag{2.19}$$

where the subscript in Δ_x indicates that the Laplacian is acting on the x variables. Let us differentiate under the integral sign, use (2.18), and collect powers of $\hbar$. One can show that the leading order equation does not involve a; it's the time-dependent Hamilton-Jacobi equation for S:

$$H(x,\nabla_x S(t,x,p)) \;=\; \frac{1}{2}\,\|\nabla_x S(t,x,p)\|^2 + V(x) \;=\; -\frac{\partial}{\partial t}\,S(t,x,p). \tag{2.20}$$

(In the language of geometrical optics this is sometimes also called the eikonal equation.) We have yet to impose the initial condition: $U(0,x,y)=\delta(x-y)$, the Schwartz kernel of the identity operator. Given the form of the phase in (2.17), by the Fourier inversion theorem this is achieved if we take

$$S(0,x,p) \;=\; x\cdot p \tag{2.21}$$

and

$$a(0,x,y,p,\hbar) \;=\; \frac{1}{(2\pi)^n}. \tag{2.22}$$

The problem (2.20, 2.21) indeed has a solution, for small $|t|$. (One of the technical difficulties in the proof of Theorem 2.2 is obtaining an ansatz for U for $|t|$ large. We won't address this problem here.)

The leading term of the amplitude, $a_0(t,x,y,p)$, satisfies the subprincipal (with respect to $\hbar$) equation obtained by writing (2.19) under the integral sign. This equation, called the transport equation, is complemented by the initial condition (2.22). One can show that all transport equations can be solved for $|t|$ small.

Having found an ansatz one applies the method of stationary phase to (2.16), that is, to the integral

$$\int e^{i\hbar^{-1}[S(t,x,p)-x\cdot p+tE]}\, a(t,x,x,p,\hbar)\, \check{\varphi}(t)\, dx, dt\, dp. \tag{2.23}$$

We need to compute the critical points of the phase, ϕ, with respect to the integration variables. Let us list the equations we get:

$\partial_t\phi = 0$: This is equivalent to: $-\frac{\partial}{\partial t}S(t,x,p) = E$. In view of the Hamilton-Jacobi equation, this is equivalent to:

$$H(x, \nabla_x S(t,x,p)) = E. \tag{2.24}$$

$\nabla_p\phi = 0$:

$$\nabla_p S(t,x,p) = x. \tag{2.25}$$

$\nabla_x\phi = 0$:

$$\nabla_x S(t,x,p) = p. \tag{2.26}$$

At this point one needs the following result from Mechanics:

Proposition 2.1. *Let S be a solution to the problem (2.20, 2.21). Then if $\{\Phi_t\}$ denotes the Hamilton flow of H one has:*

$$\Phi_t(x, \nabla_x S(t,x,p)) = (\nabla_p S(t,x,p), p). \tag{2.27}$$

The conclusion of our analysis is the following: *The critical points of the phase correspond precisely to the points $(x,p) \in \mathbb{R}^{2n}$ of phase space and numbers $t \in \mathbb{R}$ such that*

$$H(x,p) = E \qquad \text{and} \qquad \Phi_t(x,p) = (x,p).$$

This shows that the asymptotics of (2.6) arise precisely from the periodic trajectories of the Hamilton flow of H on the energy surface Σ_E.

Remarks. We can now make some very general comments as to where the terms appearing in (2.13) come from:

1. The Liouville measure of Σ_E arises as the contribution of the critical points $t=0$, $(x,p) \in \Sigma_E$. These critical points are not isolated and therefore are degenerate, and therefore Theorem (B.4) does not apply immediately. However, the manifold

$$\mathcal{C} = \{\,(0,x,p) \in \mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n \ ;\ (x,p)\in\Sigma_E\,\}$$

is a non-degenerate manifold of critical points for the phase, meaning that the *normal hessian* of the phase at each point of $\mathcal{C}$ is non-degenerate. One can then do stationary phase in the normal direction and end up with an integral along $\mathcal{C}$, which yields $\mathrm{LVol}(\Sigma_E)$. (See the remarks at the end of Appendix B.)

2. The factor $e^{i\hbar^{-1}\oint_\gamma p dx}$ is the value of the phase of the integral (2.23) at the critical point given by γ, see Appendix C ((C.20)).

3. The factor $e^{\pi i \mu_\gamma/4}$ corresponds to the factor $e^{i\pi\sigma/4}$ in the method of stationary phase, (c.f.B.4), that is μ_γ is the signature of the Hessian of the phase at the critical point given by γ.

4. The coefficient $\dfrac{T_\gamma^\sharp}{\sqrt{|\det(I-P_\gamma)|}}$ is very roughly $\dfrac{1}{\sqrt{|\mathrm{Hess}_\gamma(S)|}}$, where Hess denotes the Hessian. (Comments similar to those of 1. above apply.)

3. Special cases, generalizations.

There exist many special cases, and generalizations of the semi-classical trace formula, and in this final section I will review a couple of them. I will not attempt to sketch most of the proofs, but simply refer to the literature.

3.1. The periodic case. Consider once again a Schrödinger operator, $P_\hbar = -\hbar^2\Delta + V$, on $L^2(\mathbb{R}^n)$ (or on a compact n-dimensional Riemannian manifold), and the associated classical Hamiltonian: $H(x,p) = \frac{1}{2}\|p\|^2 + V(x)$. (More generally, one can consider an $\hbar$-pseudodifferential operator with symbol H and subprincipal symbol equal to zero.) Assume that the level sets of H are compact; then, for $\hbar$ sufficiently small, the spectrum of $P_\hbar$ is discrete. Let us suppose that for some $E \in \mathbb{R}$, a regular value of H, the classical flow on $\Sigma_E = H^{-1}(E)$ is *periodic.* It is known that the (smallest) period of the trajectories on Σ_E does not have to be constant, so the periodicity assumption needs to be clarified. Specifically, let us assume that there exists a smooth function,

$$T : \Sigma_E \to \mathbb{R}^+,$$

such that: $\forall (x,p) \in \Sigma_E$ the classical trajectory through (x,p) is periodic, with smallest (positive) period $T(x,p)$. As stated, the trace formula of the previous section does not apply, but one can still raise the question: what is the semi-classical behavior of the spectrum of $P_\hbar$ in a neighborhood of E of size $O(\hbar)$?

Before giving some answers to this question, let us recall a Theorem from classical mechanics: In the situation above, all trajectories on Σ_E have the same (Maupertuis) action:

Lemma 3.1. *Let $\phi_t : \Sigma_E \to \Sigma_E$ denote the classical flow restricted to Σ_E, and denote: $\gamma_{(x_0,p_0)} = \{\, \phi_t(x_0,p_0)\ ;\ 0 \le t \le T(x_0,p_0)\,\}$ the trajectory through $(x_0,p_0) \in \Sigma_E$. Then*

$$A := \int_{\gamma_{(x_0,p_0)}} p\, dx$$

is independent of $(x_0,p_0) \in \Sigma_E$.

For the proof we refer to [**11**], pg. 167. The Maslov index, μ, of $\gamma_(x_0,p_0)$ is likewise independent of $(x_0,p_0) \in \Sigma_E$. With this in mind, we can state the first result, as follows:

PROPOSITION 3.1. *In the previous situation, for each test function φ such that $\check{\varphi} \in C_0^\infty(\mathbb{R})$, one has an asymptotic expansion:*

(3.1)
$$\sum_j \varphi\left(\frac{E_{j,\hbar} - E}{\hbar}\right) \sim \hbar^{1-n} \sum_{k\in\mathbb{Z}} e^{ik\hbar^{-1}A}\, e^{ik\mu\pi/4} \int_{\Sigma_E} (\check{\varphi} \circ kT)\, dL + O(\hbar^{2-n}),$$

where dL is Liouville measure on Σ_E.

This result can be related to the discussion of the previous section: When one applies the method of stationary phase to the semi-classical propagator, one finds that the critical points consist of the manifold

$$\mathcal{P} = \bigcup_{k\in\mathbb{Z}} \{(w,t) \in \Sigma_E \times \mathbb{R}\ ;\ t = kT(w)\,\}.$$

Each of the connected components of this manifold has the same dimension, $2n-1$, and therefore contributes to the leading coefficient of the stationary phase expansions. The index, k, labels the iterates of each primitive trajectory, $\gamma_{(x_0,p_0)}$. The resulting leading coefficient is a clear generalization of that of Theorem 2.2.

The previous result suggests to consider the case when the period function, T, is a constant, and to restrict the values of $\hbar$ to the sequence

$$\hbar = \frac{A}{l}, \quad l = 1, 2, \ldots \tag{3.2}$$

We will say that $\hbar$'s of the form (3.2) are of *Bohr-Sommerfeld form*. For such $\hbar$ the oscillatory terms in (3.1) become one, and if furthermore T is constant, the leading term in the expansion (3.1) is simply:

$$\hbar^{1-n}\ \mathrm{LVol}(\Sigma_E) \sum_{k\in\mathbb{Z}} e^{ik\mu\pi/4}\, \check{\varphi}(kT).$$

This sum can be evaluated using the Poisson summation formula, since

$$e^{ik\mu\pi/4}\, \check{\varphi}(kT) = \check{\varphi_\mu}(kT)$$

where $\check{\varphi_\mu}(t) = e^{it\mu\pi/(4T)}$ is the inverse Fourier transform of the function

$$\varphi_\mu(\lambda) = \varphi\left(\lambda + \frac{\mu\pi}{4}\right).$$

One obtains, for $\hbar$ of Bohr-Sommerfeld form:

$$\sum_j \varphi\left(\frac{E_{j,\hbar} - E}{\hbar}\right) \sim \hbar^{1-n}\ \mathrm{LVol}(\Sigma_E) \sum_{k\in\mathbb{Z}} \varphi\left(k\frac{2\pi}{T} + \frac{\mu\pi}{4}\right). \tag{3.3}$$

Notice that φ appears on both sides of this relation. This result indicates that for $\hbar$ of the Bohr-Sommerfeld form, the spectrum of $P_\hbar$ near E is close to the points along the arithmetic sequence $2\pi k/T + \mu\pi/4$. To see this, proceed, heuristically, as follows. For a given integer k_0, take φ identically equal to one near $k_0\frac{2\pi}{T} + \pi\mu/4$ and supported near that point, so that the right-hand side is simply $\hbar^{1-n}$ $\mathrm{LVol}(\Sigma_E)$. (This is heuristic, because the Theorem stated above does not include such test functions.) The left-hand side of (3.3) is then a sum over j's such that

$$\left|\frac{E_{j,\hbar} - E}{\hbar} - \left(k_0\frac{2\pi}{T} + \frac{\mu\pi}{4}\right)\right| < c,$$

for some small $c > 0$. For any k_0, asymptotically, as $\hbar \to 0$ along Bohr-Sommerfeld values, the number of such j is $\hbar^{1-n}$ LVol(Σ_E).

In fact, part of the spectrum of $P_\hbar$ actually *clusters* tightly about this sequence. The Theorem is as follows:

THEOREM 3.2. [**5**], [**6**] *Suppose the period function $T : \Sigma_E \to \mathbb{R}^+$ is constant. Then there exist positive constants, C_1 and C_2, such that for $\hbar$ of the form (3.2) and small enough*

$$\{ j \; ; \; |E_j - E - \hbar\pi\mu/4T| < \hbar C_1 \} = \{ j \; ; \; |E_j - E - \hbar\pi\mu/4T| < \hbar^2 C_2 \} \tag{3.4}$$

In fact more is true: one can refine the analysis of the part of the spectrum singled out by the previous theorem, at a finer scale. Consider the compact manifold $Y = \Sigma_E/T\mathbb{Z}$, quotient of the energy surface Σ_E by the classical flow. Then Y is naturally a symplectic manifold: it has a symplectic structure, σ, characterized by the fact that if $\pi : \Sigma_E \to Y$ is the natural projection, then $\pi^*\sigma$ is the pull-back of $\sum dp \wedge dx$ to Σ_E. One can then show that there exists a "spectral density function",

$$\delta : Y \to \mathbb{R},$$

such that: If $\mathcal{I}$ is the set of indices in (3.4), one has: $\forall f \in C(\mathbb{R})$

$$\frac{1}{|\mathcal{I}|} \sum_{j \in \mathcal{I}} f\left(E_j - E - \hbar\pi\mu/4T\right) \sim \frac{1}{\text{Vol } Y} \int_Y f \circ \delta \, \frac{\sigma^{n-1}}{(n-1)!}.$$

Here $|\mathcal{I}|$ is the cardinality of the index set, $\mathcal{I}$, and is a polynomial in $l = A/\hbar$ closely related to the Riemann-Roch polynomial of Y. The calculation of δ is a fairly challenging problem.

It should be said that in case $n = 1$ the periodicity assumption is automatic, although one in general has the complication that Σ_E is non-connected and T is only locally constant. Nevertheless, the results above are more or less equivalent to the classical Bohr-Sommerfeld quantization condition. In this lowest dimension the set $\mathcal{I}$ eventually contains finitely-many elements, as many as the connected components of Σ_E.

3.2. The spectrum near critical values. In all the previous Theorems the assumption was made that E is a regular value of H. This is equivalent to assuming that there are not any points of equilibrium of the classical system with energy equal to E. This assumption can be dropped, provided one replaces it with assumptions on the critical points of H on Σ_E. The main complication one faces is that the trace one wants to estimate is given by an oscillatory integral with a phase function that has *degenerate* critical points. One can extend the method of stationary phase to such integrals, but in general the problem is a good deal more complicated. (Indeed just the classification of degenerate critical points of a phase function is non-trivial.) An analysis of this sort was carried out in [**4**]; here I will just quote a special case of the results obtained therein.

Let

$$\Theta = \{ w \in \Sigma_E \; ; \; dH_w = 0 \}$$

denote the set of critical points in Σ_E. Clearly, $\Sigma_E \setminus \Theta$ is a submanifold. In [**4**] we considered the case when Θ itself is a submanifold, and furthermore at each $w \in \Theta$ the Hessian of H at w normal to Θ is non-degenerate. The simplest such situation is when Θ is exactly one point, and H has a non-degenerate Hessian at that point.

THEOREM 3.3. *Assume Θ is exactly a point. Let ν denote the number of negative eigenvalues of the Hessian of H at Θ. Then, for every smooth function with compactly supported Fourier transform, φ:*

1. *If ν is odd there is an asymptotic expansion*

$$\sum_j \varphi\left(\frac{E_{j,\hbar}-E}{\hbar}\right) \sim \hbar^{1-n} \sum_{j=0}^{\infty} \sum_{l=0,1} c_{j,l}\, \hbar^j\, [\log(1/\hbar)]^l \tag{3.5}$$

   involving logarithms of $\hbar$. Moreover, the first non-zero coefficient involving such a logarithm, $c_{j_0,1}$, occurs for $j_0 = n-1$. In particular, if $n = 1$ the leading order term is of the order of $\log(1/\hbar)$.
2. *If ν is even, there is an asymptotic expansion*

$$\sum_j \varphi\left(\frac{E_{j,\hbar}-E}{\hbar}\right) \sim \hbar^{1-n} \sum_{j=0}^{\infty} c_j\, \hbar^{j/2}$$

   involving, in general, half-integer powers of $\hbar$.
3. *If $n > 1$ then in every case the leading coefficient of the expansion is the same as in the regular case.*

The case: $n = 1$ and $\nu = 1$, i.e. a saddle point in one degree of freedom, was treated independently by Bleher, [**3**]. Since the leading term in (3.5) is of the order of $\log(1/\hbar)$, the Weyl law changes: The eigenvalue counting function

$$N_c(\hbar) = \{\, j\ ;\ |E_j(\hbar) - E| \leq c\hbar\,\}$$

satisfies:

$$N_c(\hbar) \sim c\mu(\Theta)\log(\hbar^{-1}), \tag{3.6}$$

where $\mu(\Theta)$ is a certain "measure" of Θ. This result is in agreement with the following general uncertainty principle: one can place one semiclassical state per unit volume of phase space, measured in units of $(2\pi\hbar)^n$. In the current situation, this suggests that one ought to have

$$2\pi\hbar\, N(\hbar) \sim \text{Area of } H^{-1}[E - \hbar c\,,\, E + \hbar c].$$

One can check that indeed this yields (3.6).

Analytically, to treat the case $n = 1$ and $\nu = 1$, one must estimate, as $\tau \to \infty$, an integral of the form

$$\int_{\mathbb{R}^3} e^{i\tau\, s(x^2-y^2)}\, a(s,x,y)\, ds\, dx\, dy$$

where a is smooth and compactly supported. This is a beautiful, fairly elementary, analytical problem; see [**4**] for details.

Appendix A. The Fourier transform

A.1. Basic results. We begin by defining the FT on $C_o^\infty(\mathbb{R}^n)$, the space of smooth compactly-supported functions on $\mathbb{R}^n$:

DEFINITION A.1. If $f \in C_o^\infty(\mathbb{R}^n)$, we define:

$$\hat{f}(\xi) = \int e^{-ix\cdot\xi}\, f(x)\, dx.$$

The definition makes sense for $f \in L^1$, and:

LEMMA A.2. *If $f \in L^1$ then $\hat{f}$ is a continuous function such that* $\forall \xi$

$$|\hat{f}(\xi)| \leq \|f\|_{L^1}. \tag{A.1}$$

PROOF. The bound above is obvious, and continuity is justified by the dominated convergence theorem. ☐

Notation:

$$D_j \,=\, \frac{1}{i}\frac{\partial}{\partial x_j}\,, \quad D^\alpha \,=\, D_1^{\alpha_1}\cdots D_n^{\alpha_n}$$

where $\alpha = (\alpha_1, \dots, \alpha_n)$ is a multi-index. We also let $\xi^\alpha = \xi_1^{\alpha_1}\cdots\xi_n^{\alpha_n}$.

Some basic properties of the FT:

LEMMA A.3. $\forall f,\, g \in C_o^\infty(\mathbb{R}^n)$ *and all multi-indices* α,

1. $\widehat{D^\alpha f}(\xi) = \xi^\alpha\, \hat{f}(\xi)$,
2. $\widehat{x_j f}(\xi) = i\dfrac{\partial}{\partial \xi_j}\hat{f}$,
3. $\displaystyle\int \hat{f}(y)\, g(y)\, dy = \int f(x)\, \hat{g}(x)\, dx.$

The proof is very easy, just integrate by parts for 1 and 2, and apply Fubini to get 3.

COROLLARY A.4. $\forall f \in C_o^\infty(\mathbb{R}^n)$ *one has:*

$$\forall\, \alpha,\, \beta \quad \sup |\xi^\alpha\, D_\xi^\beta \hat{f}(\xi)| < \infty. \tag{A.2}$$

To prove this apply repeatedly the first two items of Lemma A.3 and (A.1).

The previous result motivates the following definition:

DEFINITION A.5. The space of Schwartz functions on $\mathbb{R}^n$, denoted $\mathcal{S}(\mathbb{R}^n)$, consists of all smooth functions on $\mathbb{R}^n$ such that

$$\forall\, \alpha,\, \beta \quad \|f\|_{\alpha,\beta} \,:=\, \sup |x^\alpha\, D_x^\beta f(x)| < \infty. \tag{A.3}$$

Obviously $C_o^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$, but for example a function of the form

$$f(x) \,=\, p(x)\, e^{-|x|^2/2}$$

where p is a polynomial is in $\mathcal{S}(\mathbb{R}^n)$ but not in $C_o^\infty(\mathbb{R}^n)$.

With this terminology Corollary A.4 states that the Fourier transform maps $C_o^\infty(\mathbb{R}^n)$ into $\mathcal{S}(\mathbb{R}^n)$. The same argument also shows that the FT maps $\mathcal{S}(\mathbb{R}^n)$ into itself. We will soon prove the following Theorem:

THEOREM A.6. *The Fourier transform is a bijection of $\mathcal{S}(\mathbb{R}^n)$ onto itself; its inverse is*

$$\check{g}(x) \,=\, \frac{1}{(2\pi)^n}\int e^{ix\cdot\xi}\, g(\xi)\, d\xi.$$

There are several different proofs of this Theorem; the one we will give exploits part (3) of Lemma A.3 with g a Gaussian. We first need to compute the Fourier transform of a Gaussian. We will do so in slightly greater generality than needed, for future reference.

PROPOSITION A.1. *Let A be a symmetric positive-definite $n \times n$ matrix, and let*

$$g_A(x) \;=\; e^{-x\cdot Ax/2}.$$

(Think of x as a column vector, so that $x \mapsto x \cdot Ax$ is the quadratic form defined by A.) Then the FT of g_A is:

$$\widehat{g_A}(\xi) \;=\; \frac{(2\pi)^{n/2}}{\sqrt{\det A}}\, g_{A^{-1}}(\xi).$$

PROOF. Without loss of generality we can assume A to be diagonal, and then it suffices to prove the result for $n = 1$, that is for

$$g_a(x) = e^{-ax^2/2}, \quad a > 0.$$

(EXERCISE: Verify this claim.) Notice that g_a satisfies the equation: $g_a' = -ax\, g_a$. Dividing by i and applying the FT to both sides we get (using Lemma A.3)

$$\xi\, \widehat{g_a}(\xi) \;=\; -a\, (\hat{g_a})'(\xi).$$

Any solution of this equation is of the form $\widehat{g_a}(\xi) = C^{-\xi^2/(2a)}$, where $C = \widehat{g_a}(0) = \int g_a(x) dx$. A well-known calculation gives $\int e^{-ax^2/2}\, dx \;=\; \sqrt{2\pi/a}$, and the result follows. □

PROOF OF THEOREM A.6. Apply part 3 of Lemma A.3 with $g = g_{aI} = \exp(-a|x|^2/2)$, to get:

$$\frac{(2\pi)^{n/2}}{a^{n/2}} \int f(x)\, e^{-|x|^2/2a}\, dx \;=\; \int \hat{f}(y)\, e^{-a|y|^2/2}\, dy\,. \tag{A.4}$$

We now let $a \to 0$. On the RHS the integrand tends to $\hat{f}$, and by Lebesgue dominated the integral converges to $\int \hat{f}(y)\, dy$. To see what happens to the LHS in the limit, make the change of variables $u = \frac{1}{\sqrt{a}} x$ to get that the LHS equals

$$(2\pi)^{n/2} \int f(\sqrt{a}u)\, e^{-|u|^2/2}\, du.$$

As $a \to 0$ once again Lebesgue dominated yields that the limit is $(2\pi)^n\, f(0)$. Thus we have shown that

$$f(0) \;=\; \frac{1}{(2\pi)^n} \int \hat{f}(\xi)\, d\xi. \tag{A.5}$$

This is the inversion formula at $x = 0$. To obtain it in general proceed as follows. Given $w \in \mathbb{R}^n$ let

$$f_w(x) \;=\; f(x + w). \tag{A.6}$$

Obviously $f_w \in \mathcal{S}(\mathbb{R}^n)$, and therefore we can apply (A.5) to it. The FT of f_w is easily computed (proof left as an exercise) and Theorem A.6 follows:

LEMMA A.7. *Let $f \in \mathcal{S}(\mathbb{R}^n)$, $w \in \mathbb{R}^n$ and define f_w by (A.6). Then*

$$\widehat{f_w}(\xi) \;=\; e^{iw\cdot\xi}\, \hat{f}(\xi).$$

COROLLARY A.8. . *Let $f, g, \in \mathcal{S}(\mathbb{R}^n)$, and let $< f, g >= \int f(x)\overline{g(x)} dx$ denote the L^2 inner product. Then (Parseval's identity)*

$$< f, g >= \frac{1}{(2\pi)^n} < \hat{f}, \hat{g} > .$$

In particular (Plancherel's identity)

$$\|f\|_2 \;=\; \frac{1}{(2\pi)^{n/2}}\,\|\hat{f}\|_2.$$

PROOF. Set

$$h \;:=\; \frac{1}{(2\pi)^n}\,\overline{\hat{g}}.$$

so that the RHS of Parseval's identity is $\int \hat{f}(x)h(x)dx$. Now use part 3 of Lemma A.3, applied to f and h. The Fourier inversion formula implies that $\overline{\hat{h}} = g$. □

A.2. An application. As an application we can solve the wave equation on $\mathbb{R}^n$: Find a function $u(t,x)$ that is e.g. smooth and Schwartz in the x variables such that

$$\frac{\partial^2 u}{\partial t^2} \;=\; \Delta(u), \tag{A.7}$$

where $u(0,x)$ and $\frac{\partial u}{\partial t}(0,x)$ are given. Here $\Delta = \sum \partial^2/\partial x_j^2$ is the Laplacian. Let us solve a particular case of this problem (that actually turns out to be sufficient for solving the general problem), namely:

$$i\frac{\partial u}{\partial t} \;=\; \sqrt{-\Delta}\,(u), \tag{A.8}$$

where $u(0,x)$ is given. Here $\sqrt{-\Delta}$ is the operator defined by:

$$\sqrt{-\Delta}\,(f) \;=\; [\|\xi\|\hat{f}(\xi)]\check{}. \tag{A.9}$$

(It is easy to see that $\sqrt{-\Delta}$ maps $\mathcal{S}(\mathbb{R}^n)$ into itself and its square is indeed $-\Delta$.) Notice that indeed (A.8) implies (A.7). To solve (A.8) for each t perform a Fourier transform in x: Let

$$f(t,\xi) \;:=\; \int e^{-ix\cdot\xi}\,u(t,\xi)\,d\xi.$$

Then the equation becomes

$$i\frac{\partial f}{\partial t}(t,\xi) \;=\; \|\xi\|\,\hat{f}(t,\xi).$$

This can be solved immediately: $f(t,\xi) = e^{-it\|\xi\|}\,f(0,\xi)$. Applying the inverse Fourier transform one obtains that the solution to (A.8) is

$$u(t,x) \;=\; \frac{1}{(2\pi)^n}\int e^{i[x\cdot\xi - t\|\xi\|]}\,f_0(\xi)\,d\xi \tag{A.10}$$

where f_0 is the Fourier transform of the initial condition, $u_0 = u|_{t=0}$. In terms of u_0 itself the solution is

$$u(t,x) \;=\; \frac{1}{(2\pi)^n}\int\!\!\int e^{i[(x-y)\cdot\xi - t\|\xi\|]}\,u_0(y)\,dy\,d\xi. \tag{A.11}$$

Appendix B. The method of stationary phase

The method of stationary phase is the name given to a collection of old results on the asymptotic behavior of integrals of the form

$$I(\tau) \;=\; \int_{\mathbb{R}^n} e^{i\tau\phi(x)}\, a(x)\, dx \tag{B.1}$$

where ϕ is smooth and for simplicity we take $a \in C_o^\infty(\mathbb{R}^n)$ and independent of τ. ϕ is called the phase and a the amplitude. We will choose ϕ to be real-valued. The problem is to estimate (B.1) as $\tau \to \infty$. Notice the obvious bound

$$|I(\tau)| \leq \|a\|_{L^1}, \tag{B.2}$$

but $I(\tau)$ may well be smaller. As a warm-up let's look at two extreme cases.

1. Suppose ϕ is constant: $\phi(x) = c$. Then
$$I(\tau) \;=\; e^{i\tau c} A,$$
where A is a constant (i.e. independent of τ). Therefore $I(\tau)$ oscillates but $|I(\tau)|$ is a constant. This shows that the obvious bound (B.2) is optimal in general.
2. Suppose ϕ is a coordinate function, say $\phi(x) = x_1$. Then
$$I(\tau) \;=\; \hat{a}(-\tau, 0, \dots, 0).$$
Since a is smooth compactly supported $\hat{a}$ is Schwartz, and therefore in this case
$$\forall N > 0 \qquad I(\tau) \;=\; O(\tau^{-N}).$$

Intuitively, in case 2 we obtain rapid decrease because for large τ the exponential $\exp(i\tau\phi(x))$ oscillates many times between x and $x + dx$, while the amplitude $a(x)$ remains relatively constant (since a is smooth). Therefore in the sum (integral) many cancellations take place. This is clearly the opposite of what happens in case 1. If ϕ has a critical point x_0, i.e. if $d\phi_{x_0} = 0$, then between x_0 and $x_0 + dx$ the phase ϕ doesn't change very much, so infinitesimally we are in case 1. Therefore we expect that in general the main contributions to $I(\tau)$ should arise from the critical points of ϕ, that is points where ϕ is "stationary". This is indeed the case.

General references for this material are [**7**], section 1.2 and [**14**], section 7.7.

B.1. Non-stationary phases. First we show that the main contribution arise from the critical points of the phase in the support of the amplitude.

Proposition B.1. *Let* $I(\tau) \;=\; \int_{\mathbb{R}^n} e^{i\tau\phi(x)}\, a(x)\, dx$ *where* $a \in C_o^\infty(\mathbb{R}^n)$ *and* ϕ *is smooth. Assume that* ϕ *doesn't have any critical points in a neighborhood of the support of* a*. Then*

$$\forall N > 0 \qquad I(\tau) \;=\; O(\tau^{-N}).$$

Proof. The idea is to use the identity:

$$\nabla\phi\left(e^{i\tau\phi(x)}\right) \;=\; i\tau\|\nabla\phi\|^2 e^{i\tau\phi(x)}$$

and to integrate by parts. Here on the left-hand side $\nabla\phi$ is considered as the differential operator

$$\nabla\phi \;=\; \sum_{j=1}^{n} \frac{\partial\phi}{\partial x_j}\,\frac{\partial}{\partial x_j}.$$

Let χ be a smooth cut-off function identically one on the support of a and such that $\nabla\phi$ does not vanish on its support. Therefore $a\chi = a$, and $\chi/\|\nabla\phi\|^2$ is a smooth function. Let

$$L := \frac{\chi}{\|\nabla\phi\|^2} \sum_{j=1}^{n} \frac{\partial\phi}{\partial x_j} \frac{\partial}{\partial x_j}.$$

This is a smooth vector field satisfying

$$L\, e^{i\tau\phi(x)} = i\tau\,\chi\, e^{i\tau\phi(x)},$$

and therefore

$$a\, e^{i\tau\phi(x)} = a\,\chi\, e^{i\tau\phi(x)} = \frac{a}{i\tau}\, L\, e^{i\tau\phi(x)}.$$

Therefore

$$I(\tau) = \int \frac{a}{i\tau}\, L\, e^{i\tau\phi(x)}\, dx = \frac{i}{\tau} \int e^{i\tau\phi(x)}\, L^t a\, dx. \tag{B.3}$$

Here L^t is the transpose of L. Applying the bound (B.2), we get:

$$|I(\tau)| \le \frac{1}{|\tau|}\, \|L^t a\|_{L^1}$$

Notice however that the right-hand side of (B.3) is of the same form as $I(\tau)$ itself (except for the factor of i/τ). Therefore the argument can be repeated any number of times. □

In applications it will be important to let both the phase and the amplitude depend on parameters, that is consider

$$I(\tau, w) = \int e^{i\tau\phi(x,w)}\, a(x,w)\, dx \tag{B.4}$$

where w ranges over some compact domain Ω in $\mathbb{R}^m$. Of course we can repeat e.g. the analysis above for each fixed w; the only question is that of the uniformity of the estimates with respect to ω.

Proposition B.2. *Assume a and ϕ are smooth. Let $K \subset \mathbb{R}^n$ be a fixed compact set such that*

$$\forall w \in \Omega,\ \forall x \notin K \qquad a(x,w) = 0$$

(i.e. for each w the support of $a(\cdot, w)$ is contained in K). Assume that

$$\{(x,w) \in K \times \Omega\,;\, \nabla_x\phi(x,w) = \vec{0}\} = \emptyset.$$

Then

$$\forall N \qquad |I(\tau,w)| = O(\tau^{-N})$$

uniformly on $w \in \Omega$.

B.2. Quadratic phases. The simplest phases with a non-degenerate critical point are the quadratic ones, $\phi(x) = x \cdot Ax/2$ where A is a real non-degenerate symmetric matrix. For such phases one has the following result:

THEOREM B.1. *If a is smooth and compactly supported, then there exists a complete asymptotic expansion*

$$\int_{\mathbb{R}^n} e^{i\tau x\cdot Ax/2}\, a(x)\, dx \sim \left(\frac{2\pi}{\tau}\right)^{n/2} \frac{e^{i\pi\sigma/4}}{\sqrt{|\det A|}} \sum_{j=0}^{\infty} \alpha_j(a)(0)\, \tau^{-j} \tag{B.5}$$

as $\tau \to \infty$, where:

1. *σ is the signature of A (the number of positive eigenvalues minus the number of negative ones).*
2. *$\alpha_0(a)(0) = a(0)$, and in general*
3. *$\alpha_j(a)$ is a differential operator of order $2j$ applied to a.*

PROOF. We can assume without loss of generality that A is diagonal, and then by a density argument (of product functions in $C_0^\infty(\mathbb{R}^n)$) it suffices to prove the result for $n = 1$. So take $A = (\Lambda)$, $\Lambda \in \mathbb{R}$. First assume that $\Lambda < 0$. By Parseval's identity and Proposition A.1, $\forall \mu > 0$

$$\int e^{\mu x^2\Lambda/2}\, a(x)\, dx = \frac{\sqrt{2\pi}}{2\pi\sqrt{-\mu\Lambda}} \int e^{y^2/2\Lambda\mu}\, \hat{a}(y)\, dy.$$

The advantage of doing this is that on the right-hand side the μ appears in the denominator. Now regard the integrals above as a function of μ. Clearly this function of μ is analytic, so one can analytically continue it to $\mu = i\tau$, $\tau > 0$, that is from the positive real semi-axis to the positive imaginary semi-axis. We simply have to take care of taking the correct analytic continuation of the square root $\sqrt{-\mu\Lambda} = \sqrt{\mu}\sqrt{|\Lambda|}$ (recall that we are assuming $\Lambda < 0$). This leads to the identity

$$\int e^{i\tau x^2\Lambda/2}\, a(x)\, dx = \frac{1}{\sqrt{2\pi}\, e^{i\pi/4}\sqrt{\tau}\,\sqrt{|\Lambda|}} \int e^{iy^2/2\Lambda\tau}\, \hat{a}(y)\, dy.$$

This is what we had to show, i.e. it's (B.5) for the case at hand. If, on the other hand, we take $A = (\Lambda)$ with $\Lambda > 0$ then we repeat the above argument starting from $\int e^{-\mu x^2\Lambda/2}\, a(x)\, dx$. Now we have to analytically continue from the positive real semi-axis to the negative imaginary semi-axis, so we obtain a factor of $\exp -i\pi/4$ in the denominator. In conclusion one arrives at the identity

$$\int_{\mathbb{R}^n} e^{i\tau x\cdot Ax/2}\, a(x)\, dx = \frac{e^{i\pi\sigma/4}}{(2\pi)^{n/2}\,\tau^{n/2}\sqrt{|\det A|}} \int e^{iy\cdot A^{-1}y/2\tau}\, \hat{a}(y)\, dy. \tag{B.6}$$

Now do a Taylor-McLaurin expansion of the exponential and use the Fourier inversion formula. □

B.3. Non-degenerate critical points. We next consider $I(\tau)$ where the phase function, ϕ, only has non-degenerate critical points in a neighborhood of the support of the amplitude. Although it is possible to analyze $I(\tau)$ in more general cases, the non-degenerate case is by far the simplest and basically the only one we'll consider here. (See [**4**] and references therein for more information, and also the remarks at the end of this section.)

We begin by recalling the definition of a non-degenerate critical point:

DEFINITION B.2. A point $p \in \mathbb{R}^n$ is a non-degenerate critical point of $\phi : \mathbb{R}^n \to \mathbb{R}$ iff $\nabla\phi(p) = \vec{0}$ and the Hessian of ϕ at p,

$$\mathrm{Hess}_p(\phi) \;:=\; \left(\frac{\partial^2\phi}{\partial x_i \partial x_j}(p)\right)$$

is non-degenerate: $\det(\mathrm{Hess}_p(\phi)) \neq 0$.

It is known that non-degenerate critical points must be isolated (among all critical points). This is in fact implied by the following "Morse lemma", which says that near a non-degenerate critical point a function is equivalent to a quadratic function:

LEMMA B.3. *Let p be a non-degenerate critical point of a smooth function ϕ. Then there exists a neighborhood of p, W, a neighborhood of the origin in $\mathbb{R}^n$, X, and a diffeomorphism $\chi : X \to W$ such that $\chi(0) = p$ and*

$$\phi(\chi(y_1, \dots, y_n)) \;=\; \phi(p) + \frac{1}{2}\sum_{j=1}^{n} \Lambda_j y_j^2$$

where the Λ_j are the eigenvalues of $Hess_p(\phi)$. Moreover, the Jacobian of χ at the origin is one.

Combining this Lemma with Theorem B.1 and Proposition B.1, we obtain the following result:

THEOREM B.4. *Suppose that ϕ is a smooth, real-valued function on $\mathbb{R}^n$, and let $a \in C_0^\infty(\mathbb{R}^n)$. Suppose that the only critical points of ϕ in some neighborhood of the support of a are non-degenerate, and denote those in the support of a by $p_1, \dots, p_K$. Then, as $\tau \to \infty$*

$$\int e^{i\tau\phi(x)}\, a(x)\, dx \sim \left(\frac{2\pi}{\tau}\right)^{n/2} \sum_{l=1}^{K} \frac{e^{i\pi\sigma_l/4}}{\sqrt{|\det Hess_{p_l}(\phi)|}}\, e^{i\tau\phi(p_l)} \left[a(p_l) + \sum_{j=1}^{\infty} \alpha_j^l(a)(p_l)\, \tau^{-j}\right]$$

where σ_l is the signature of $Hess_{p_l}(\phi)$ and the α_j^l are differential operators.

The restriction that all critical points of the phase be non-degenerate is very restrictive. However, the following situation often occurs. Suppose the variables x split: $x = (x', x'')$ and suppose that every point along the plane $x' = 0$ is a critical point of the phase $\phi(x)$: $\nabla_x\phi(0, x'') = 0$. Suppose moreover that the Hessian in the x' variables is non-degenerate at each $(0, x'')$:

$$\det\left(\frac{\partial^2\phi}{\partial x_i' \partial x_j'}(0, x'')\right) \neq 0.$$

Clearly we can write

$$I(\tau) \;:=\; \int e^{i\tau\phi(x)}\, a(x)\, dx \;=\; \int \left(\int e^{i\tau\phi(x)}\, a(x)\, dx'\right) dx''.$$

Then we can do stationary phase on the dx' integral, for each x'', and (formally at least) integrate the resulting expansion with respect to dx'' to estimate $I(\tau)$. This in fact can be made rigorous, but I won't write the details here.

Appendix C. The Hamilton-Jacobi equation

C.1. Proof of Proposition 2.1. The goal of this section is to prove Proposition 2.1, needed to identify the critical points of the phase in the oscillatory integral (2.23). (See Arnold's book, [**1**], for general background.) Although the result is true for very general Hamiltonians, at times for simplicity we will take

$$H(x,p) \;=\; \frac{1}{2}\,\|p\|^2 + V(x). \tag{C.1}$$

Consider the Hamilton-Jacobi equation for $S = S(t,x,p)$, with the indicated initial condition:

$$\begin{cases} \frac{\partial}{\partial t} S(t,x,p) &=& -H(x, \nabla_x S(t,x,p)), \\ S(0,x,p) &=& x\cdot p. \end{cases} \tag{C.2}$$

As we will see, in these equations x *should be thought of as the initial position of a particle that after a time* t *has momentum* p. Hopefully the following results will clarify this.

Lemma C.1. *(c.f.[**2**] Theorem 5.2.4.) Suppose that a curve* $t\mapsto \tilde{x}(t)$ *in* $\mathbb{R}^n$ *satisfies the equation:*

$$\frac{d}{dt}\tilde{x}(t) \;=\; \nabla_p H(\tilde{x}(t), \nabla_x S(t,\tilde{x}(t),p_0)) \tag{C.3}$$

where $p_0\in\mathbb{R}^n$ *is fixed. Then the curve*

$$t\mapsto (\tilde{x}(t), \nabla_x S(t,\tilde{x}(t),p_0)) \tag{C.4}$$

is a trajectory of the Hamilton flow of H*.*

Proof. Notice that (C.3) is precisely one-half of Hamilton's equations for the curve (C.4). To check the other half, we compute:

$$\frac{d}{dt}\,\frac{\partial S}{\partial x_i}(t,\tilde{x}(t),p_0) \;=\; \frac{\partial^2 S}{\partial t\,\partial x_i} + \sum_j \dot{\tilde{x}}_j \frac{\partial^2 S}{\partial x_j \partial x_i} \;=$$

$$=\; \frac{\partial^2 S}{\partial t\,\partial x_i} + \sum_j \frac{\partial H}{\partial p_j}\frac{\partial^2 S}{\partial x_j \partial x_i} \tag{C.5}$$

where we have used (C.3) and all the terms in S are evaluated at $(t,\tilde{x}(t),p_0)$. On the other hand, differentiating the H-J equation ((C.2)) with respect to x_i yields

$$\frac{\partial^2 S}{\partial x_i\,\partial t}(t,x) \;=\; -\frac{\partial H}{\partial x_i}(x,\nabla_x S(t,x)) - \sum_j \frac{\partial H}{\partial p_i}\frac{\partial^2 S}{\partial x_i\,\partial p_j}.$$

Evaluating this at $(t,\tilde{x}(t))$ and substituting back into (C.3) one obtains

$$\frac{d}{dt}\,\frac{\partial S}{\partial x_i}(t,\tilde{x}(t),p_0) \;=\; -\frac{\partial H}{\partial x_i}(\tilde{x}(t),\nabla_x S(t,\tilde{x}(t))).$$

□

Remark. If H is as in (C.1), then equation (C.3) reads:

$$\frac{d}{dt}\tilde{x}(t) \;=\; \nabla_x S(t,\tilde{x}(t),p_0),$$

that is, $\forall t$ $\tilde{x}$ is normal to the level surfaces of S. This is related to Huygen's principle, see [**1**].

PROPOSITION C.1. *Let $\gamma(t) = (x(t), p(t))$ be any trajectory of the Hamilton flow of H. Then, $\forall t$*

$$p(t) = \nabla_x S(t, x(t), p(0)). \tag{C.6}$$

PROOF. We will use the fact that there is a unique trajectory with given initial conditions. Let $\tilde{x}(t)$ solve the Cauchy problem

$$\begin{cases} \frac{d}{dt}\tilde{x}(t) &= \nabla_p H(\tilde{x}(t), \nabla_x S(t, \tilde{x}(t), p(0))), \\ \tilde{x}(0) &= x(0) \end{cases} \tag{C.7}$$

and let $\tilde{\gamma}(t) = (\tilde{x}(t), \nabla_x S(t, \tilde{x}(t), p(0)))$. By Lemma C.1, $\tilde{\gamma}$ is a trajectory. It has the same initial conditions as γ, since

$$\nabla_x S(0, \tilde{x}(0), p(0)) = \nabla_x (x \cdot p(0))|_{x=\tilde{x}(0)} = p(0).$$

Therefore $\tilde{\gamma} = \gamma$. Equating p components gives (C.6). □

Let us now introduce the following notations. Let $\{\Phi_t\}$ denote the Hamilton flow of H. Denote its x and p components as follows:

$$\Phi_t(y, p_0) = (x(t, y, p_0), p(t, y, p_0)). \tag{C.8}$$

We will assume that for each t and p_0 in some open set the map

$$y \mapsto x(t, y, p_0) \tag{C.9}$$

is a diffeomorphism. We will denote its inverse by

$$x \mapsto y(t, x, p_0). \tag{C.10}$$

That is, we set:

$$y(t, x, p_0) = \left(\begin{array}{c} \text{initial position of a particle} \\ \text{of initial momentum } p_0 \text{ that at time } t \text{ is at } x. \end{array} \right) \tag{C.11}$$

Alternatively, we can say that $\Phi_t(y(t, x, p_0), p_0)$ is of the form:

$$\Phi_t(y(t, x, p_0), p_0) = (x, *). \tag{C.12}$$

With these notations we can re-state (C.6) as follows:

COROLLARY C.2.

$$\forall t,\ x,\ p \qquad \Phi_t(y(t, x, p), p) = (x, \nabla_x S(t, x, p)).$$

We can now prove Proposition 2.1; let's restate it for convenience:

PROPOSITION C.2. *Let S be a solution to the problem (C.2). Then*

$$\Phi_t(x, \nabla_x S(t, x, p)) = (\nabla_p S(t, x, p), p). \tag{C.13}$$

PROOF. By virtue of the previous Corollary all we need to show is that $\forall t,\ x,\ p$

$$y(t, x, p) = \nabla_p S(t, x, p). \tag{C.14}$$

Equivalently, for each t, p let us substitute in this equation x for $x = x(t, y, p)$ (where y here is regarded as an independent variable). Since (C.9, C.10) are inverses of each other, equation (C.14) becomes

$$\forall t,\ y,\ p \qquad y = \nabla_p S(t, x(t, y, p), p). \tag{C.15}$$

This equation holds for $t = 0$ (since $x(0, y, p) = y$ and $S(0, x, p) = x \cdot p$). Let us now differentiate the right-hand side with respect to t: □

C.2. Relation with the action functional. We will now see that the solution, S, to the Hamilton-Jacobi equation is closely related to the action functional, which accounts for the presence of the term $\int_\gamma pdx$ in the STF (Theorem 2.2).

We begin with some concepts from Mechanics, see for example [**1**], [**2**] for details. We'll restrict ourselves to the case of a Hamiltonian, H, of the form (kinetic energy) + (potential) except that in this case we will introduce, for conceptual clarity, the mass m of the particle. Let us begin with the Lagrangian density,

$$L(x,v) := \frac{m}{2}\|v\|^2 - V(x), \tag{C.16}$$

where $v \in \mathbb{R}^n$ is in fact a tangent vector representing a possible velocity of the particle. The momenta associated to L are defined in general by:

$$p_j := \frac{\partial L}{\partial v}$$

which in this case simply amounts to:

$$p = mv.$$

(Abstractly, these equations define the diffeomorphism $(x,v) \mapsto (x,p)$ between the tangent and cotangent bundles of configuration space, the Legendre transformation.) The Hamiltonian is related to the Lagrangian density by the relation

$$H(x,p) = p\cdot v - L(x,v) = m\|v\|^2 - \frac{m}{2}\|v\|^2 + V(x),$$

which, after substituting $v = p/m$, yields

$$H(x,p) = \frac{1}{2m}\|p\|^2 + V(x).$$

Although we have taken $m = 1$ and therefore $p = v$, it is important to understand that p and v are of different nature.

The following holds for all values of m (and more general Lagrangians):

Lemma C.3. *Let $S(t,x,p)$ satisfy the equations (C.2). Then, if $(x(t),p(t))$ is any trajectory of the Hamilton flow of H,*

$$\frac{d}{dt}S(t,x(t),p(0)) = L(x(t),v(t)).$$

Proof. Simply compute with the previous relations, including: the Hamilton-Jacobi equation, $\dot{x}(t) = v(t)$ and (C.6). ☐

Corollary C.4. *Under the same hypethesis as those of the previous Lemma,*

$$S(t,x(t),p(0)) = x(0)\cdot p(0) + \int_0^t L(x(s),v(s))\,ds. \tag{C.17}$$

The integral $\int_0^T L(x(s),v(s))\,ds$ is called the *action* of the trajectory $(x(t),p(t))$, $0 \le t \le T$.

Suppose $\gamma(t) = (x(t),p(t))$ is periodic of period T:

$$\gamma(t+T) = \gamma(t).$$

(Notice that we are *not* assuming that T is the minimal period of γ, i.e. γ could also be periodic of period T/k for some integer k.) Then, by (C.17), since $x(T) = x(0)$,

$$S(T,x(0),p(0)) = x(0)\cdot p(0) + \oint_\gamma L\,dt \tag{C.18}$$

(where the $\oint$ may mean integrating around γ k times if γ has minimal period T/k). However, along a trajectory,

$$Hdt = pdx - Ldt, \tag{C.19}$$

as the reader can check. Therefore

$$\oint_\gamma L\,dt = \oint_\gamma pdx - \oint_\gamma Hdt$$

Let E denote the energy of γ: $\forall t \quad H(x(t),p(t)) = E$. Therefore

$$\oint_\gamma Hdt = ET,$$

and

$$S(T,x(0),p(0)) = x(0)\cdot p(0) + \oint_\gamma pdx - TE. \tag{C.20}$$

We can now explain the presence of the factor $\oint_\gamma pdx$ in (2.13): To obtain Theorem 2.2 we are applying the method of stationary phase to the oscillatory integral (2.23) whose phase is

$$\phi(t,x,p) = S(t,x,p) - x\cdot p + tE,$$

and where the variables of integration are t, x and p. As explained in section 2.3, the critical points of this phase (with respect to the integration variables) are precisely the $(T,x(0),p(0))$ where the trajectory with initial condition $(x(0),p(0))$ is periodic of period T and $H(x(0),p(0)) = E$. By (C.20), the value of the phase at such a point is

(C.21)

$$\phi(T,x(0),p(0)) = x(0)\cdot p(0) + \oint_\gamma pdx - TE - x(0)\cdot p(0) + TE = \oint_\gamma pdx.$$

References

[1] V.I Arnol'd, *Mathematical methods of classical mechanics*, Springer Verlag, 1978.

[2] Abraham and Marsden, *Foundations of Mechanics* Benjamin-Cummings, 1978.

[3] P. M. Bleher. Semiclassical quantization rules near separatrices. Comm. Math. Phys. **165** No. 3, 621-640, (1994).

[4] R. Brummelhuis, T. Paul and A. Uribe. Spectral estimates around a critical level, Duke Math. J. 78 No.3, 477-530 (1995).

[5] R. Brummelhuis and A.Uribe. A semiclassical trace formula for Schrödinger operators, Comm. Math. Phys., **136**, 567-584, (1991).

[6] S. Dozias. Clustering for the spectrum of $\hbar$-pseudodifferential operators with periodic flow on an energy surface, J. of Funct. Analysis **145** (1997), 296-311.

[7] J.J. Duistermaat. *Fourier integral operators*, Birkhauser, Boston 1996.

[8] J.J. Duistermaat and V. Guillemin. The spectrum of positive elliptic pseudodifferential operators and periodic bicharacteristics, Inventiones Math. **29** 39-79 (1975).

[9] Dym and McKean. *Fourier series and integrals.* Academic Press, 1972.

[10] M. Gutzwiller: Periodic orbits and classical quantization conditions, J. Math. Phys. **12**, (1971), 343-358. See also: *Chaos in Classical and Quantum Mechanics*, Interdisciplinary Applied Mathematics Vol. 1, Springer Verlag, 1990.

[11] V. Guillemin and S. Sternberg. *Geometric Asymptotics* Math. Surveys No. 14, Amer. Math. Soc., Providence R.I. 1977.

[12] V. Guillemin and A. Uribe. Circular symmetry and the trace formula, Invent. Math., **96**, 385-423, (1989).

[13] B. Helffer. $\hbar$-Pseudodifferential operators and applications: an introduction. In *Quasiclassical Methods*, J. Rauch and B. Simon, Editors. Spinger, 1997.

[14] L. Hörmander. *The analysis of linear partial differential operators, I.* Springer-Verlag.
[15] E. Meinrenken. Semiclassical principal symbols and Gutzwiller's trace formula, Reports on Mathematical Physics Vol 31 p.279-295.
[16] T. Paul and A. Uribe. Sur la formule semi-classique de traces, Comptes Rendus de l'Academie de Sciences, Paris, **313** (Ser. I) 217-222 (1991).
[17] T. Paul and A. Uribe. The semi-classical trace formula and propagation of wave packets, J. Funct. Analysis **132** No.1, 192-249 (1995).
[18] M. Reed and B. Simon. *Methods of Modern Mathematical Physics I: Functional Analysis.* Academic Press, 1980.

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