

# Introducción al análisis semiclásico

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# Plan del cursillo

- 1 Teoría Espectral de Operadores y Mecánica Cuántica
- 2 Cuantización y Operadores Pseudodiferenciales
- 3 Cálculo funcional para operadores pseudodiferenciales
- 4 Estudio de valores propios

# Plan de las sesiones I y II

- 1 Operadores lineales en espacios de Hilbert
- 2 Teorema Espectral (Cálculo funcional para operadores autoadjuntos)
- 3 Noción de observable cuántico, estado y ecuación de Schrödinger

# Operadores lineales en espacios de Hilbert (1)

## Definición 1

Un espacio de Hilbert  $\mathcal{H}$  es un espacio vectorial complejo, con un producto interno  $\langle \cdot, \cdot \rangle$  que es completo para la norma inducida por el producto interno  $\|f\| = \langle f, f \rangle^{\frac{1}{2}}$ , y separable.

## Comentario 1

Separable en este contexto es equivalente a tener una base numerable. Es decir que con esta definición todos los Espacios de Hilbert de dimensión infinita son isomorfos.

## Ejemplo 1

- $\mathbb{C}^n$  con  $\langle \alpha, \beta \rangle = \sum_{j=1}^n \overline{\alpha_j} \beta_j$
- $l^2(\mathbb{Z})$  con  $\langle \alpha, \beta \rangle = \sum_{n \in \mathbb{Z}} \overline{\alpha(n)} \beta(n)$
- $L^2(\mathbb{R}^n)$  con  $\langle f, g \rangle = \int_{\mathbb{R}^n} \overline{f(x)} g(x)$

# Operadores lineales en espacios de Hilbert (2)

## Definición 2

Una aplicación lineal  $B : \mathcal{H} \rightarrow \mathcal{H}$  se dice acotada (o continua) si existe  $C > 0$  tal que

$$\|Bf\| \leq C\|f\| \quad (1)$$

para todo  $f \in \mathcal{H}$ . Notamos por  $\mathcal{B}(\mathcal{H})$  el conjunto de operadores acotados en el espacio de Hilbert  $\mathcal{H}$ . Además definimos la norma,

$$\|B\| = \sup_{f \in \mathcal{H}} \frac{\|Bf\|}{\|f\|} \quad (2)$$

Además, para todo  $B \in \mathcal{B}(\mathcal{H})$  existe un único  $B^* \in \mathcal{B}(\mathcal{H})$  que satisface

$$\langle B^*f, g \rangle = \langle f, Bg \rangle . \quad (3)$$

## Operadores lineales en espacios de Hilbert (3)

Decimos que  $B^*$  es el adjunto de  $B$ . Se tiene además las siguientes propiedades.

$$\|B^*\| = \|B\| \quad ; \quad (B^*)^* = B \quad ; \quad (AB)^* = B^*A^* \quad ; \quad \|B^*B\| = \|B\|^2.$$

### Comentario 2

*Respecto de la composición de operadores,  $\mathcal{B}(\mathcal{H})$  es un álgebra. Como es completa respecto de su norma es una álgebra de Banach. Como además la involución satisface  $\|B^*B\| = \|B\|^2$  es una  $C^*$ -álgebra.*

### Proposición 1

*Todo operador acotado  $B$  se puede escribir como  $B = U|B|$  donde  $|B|$  es un operador positivo y  $U$  es un isometría parcial (isometría fuera de su kernel). Un operador positivo cumple que  $\langle f, Bf \rangle \geq 0$  y en particular es auto adjunto.*

## Algunos tipos de operadores

- $B$  es autoadjunto si  $B^* = B$
- $B$  es normal si  $B^*B = BB^*$
- $B$  es una proyección ortogonal si  $B^2 = B = B^*$
- $B$  es unitario si  $BB^* = B^*B = 1$

Consideremos  $\mathcal{H} = l^2(\mathbb{Z})$ . Si  $f : \mathbb{Z} \rightarrow \mathbb{R}$  es acotada como función, entonces el operador de multiplicación por  $f$

$$(M_f\alpha)(n) = f(n)\alpha(n) \quad (4)$$

es un operador acotado y autoadjunto. Dado cualquier vector  $g \in l^2(\mathbb{Z})$ , la proyección ortogonal en  $g$  es

$$|g\rangle\langle g|\alpha = \langle g, \alpha \rangle g . \quad (5)$$

El operador  $S$  definido por

$$(S\alpha)(n) = \alpha(n+1) \quad (6)$$

es unitario. En efecto su adjunto cumple

$$(S^*\alpha)(n) = \alpha(n-1) . \quad (7)$$

# Operadores Compactos

## Definición 3

Si el rango de un operador  $A$  es de dimensión finita decimos que es un operador de rango finito y notamos el conjunto de estos operador por  $\mathcal{F}(\mathcal{H})$ . Si  $A \in \mathcal{F}(\mathcal{H})$ , entonces existen  $\{g_j, h_j\}_{j=1}^N \subset \mathcal{H}$  tal que

$$A = \sum_{j=1}^N |h_j\rangle\langle g_j|. \quad (8)$$

## Definición 4

Decimos que  $B \in \mathcal{B}(\mathcal{H})$  es un operador compacto si es limite en norma de una sucesión de operadores de rango finito. Notamos el conjunto de los operadores compactos por  $\mathcal{K}(\mathcal{H})$ .



# Propiedades de los operadores compactos

- $B \in \mathcal{K}(\mathcal{H})$  implica  $B^* \in \mathcal{K}(\mathcal{H})$
- $A \in \mathcal{B}(\mathcal{H})$  y  $B \in \mathcal{K}(\mathcal{H})$  implica  $AB, BA \in \mathcal{K}(\mathcal{H})$
- Se tiene entonces que  $\mathcal{K}(\mathcal{H})$  es un ideal bilatero de  $\mathcal{B}(\mathcal{H})$

## Definición 5

Un operador compacto se dice de Hilbert–Schmidt si

$$\|A\|_{\mathcal{B}_2} := \sum_{j \in \mathbb{N}} \|Ae_j\|^2 < \infty \quad (9)$$

para una (cualquier) base ortonormal  $\{e_j\}_{j \in \mathbb{N}}$ . Notamos por  $\mathcal{B}_2$  la clase de operadores de Hilbert-Schmidt.

Se cumple que para todo  $B \in \mathcal{B}(\mathcal{H})$  y  $A \in \mathcal{B}_2$

$$\|AB\|_{\mathcal{B}_2} \leq \|B\| \|A\|_{\mathcal{B}_2} \quad (10)$$

# Operadores de clase traza

Para todo  $B \geq 0$  existe un único  $B^{\frac{1}{2}}$  tal que  $B^{\frac{1}{2}}B^{\frac{1}{2}} = B$ .

## Definición 6

Un operador se dice de clase traza si

$$\|A\|_{\mathcal{B}_1} := \sum_{j \in \mathbb{N}} \| |A|^{\frac{1}{2}} e_j \|^2 = \sum_{j \in \mathbb{N}} \langle e_j, |A| e_j \rangle < \infty . \quad (11)$$

Para todo  $A \in \mathcal{B}_1$  definimos

$$\mathrm{Tr}(A) = \sum_{j \in \mathbb{N}} \langle e_j, A e_j \rangle . \quad (12)$$

En resumen tenemos:

$$\mathcal{F}(\mathcal{H}) \subset \mathcal{B}_j \subset \mathcal{K}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H}) . \quad (13)$$

# Operadores (no acotados)

## Definición 7

*Un operador en un espacio de Hilbert  $\mathcal{H}$  es un par  $(A, D(A))$ , con  $D(A)$  un subespacio denso de  $\mathcal{H}$  y  $A : D(A) \rightarrow \mathcal{H}$  una aplicación lineal.*

Por ejemplo, en  $L^2((0, 1))$  el “operador”  $-i \frac{\partial^2}{\partial x^2}$  tiene diferentes dominios de interés:

- $C_c^\infty((0, 1))$  el espacio de funciones infinitamente diferenciables con soporte compacto
- El espacio de funciones infinitamente diferenciables tales que su derivadas se anulan en 0 y 1.

# Conjunto resolvente y espectro de un operador

## Definición 8

Un operador  $(A, D(A))$  es cerrado si para toda sucesión convergente de vectores  $\{f_n\}$  y tal que  $\{Af_n\}$  sea una sucesión de Cauchy, se tiene que  $\lim_{n \rightarrow \infty} f_n = f_\infty \in D(A)$  y  $\lim_{n \rightarrow \infty} Af_n = Af_\infty$

## Definición 9

Sea  $(A, D(A))$  un operador cerrado. El conjunto resolvente  $\rho(A)$  se define por

$$\rho(A) = \{z \in \mathbb{C} \mid (A - z)^{-1} \in \mathcal{B}(\mathcal{H})\} . \quad (14)$$

El operador acotado  $(A - z)^{-1} : \mathcal{H} \rightarrow D(A)$  se dice la resolvente de  $A$  en  $z$ . Se puede demostrar que  $\rho(A)$  es un conjunto abierto (de  $\mathbb{C}$ ). Se sigue que el espectro de  $A$ , definido por

$$\sigma(A) := \mathbb{C} \setminus \rho(A) \quad (15)$$

es cerrado.

## Adjunto (versión no acotada)

Dado un operador  $(A, D(A))$  su adjunto  $(A^*, D(A^*))$  se define por

$$D(A^*) = \{f \in \mathcal{H} \mid \exists f^* \in \mathcal{H} \text{ tal que } \langle f, Ag \rangle = \langle f^*, g \rangle \forall g \in D(A)\} \quad (16)$$

y  $A^*f = f^*$ .

### Lema 1

$((A^*), D(A^*))$  es un operador cerrado y  $\text{Ker}(A^*) = (\text{Ran}(A))^\perp$ .

### Definición 10

$(A, D(A))$  es autoadjunto si  $(A, D(A)) = (A^*, D(A^*))$ .

### Teorema 1

Si  $(A, D(A))$  es autoadjunto entonces  $\sigma(A) \subset \mathbb{R}$

## Definición 11

Una familia espectral es una familia de proyecciones ortogonales  $\{E_\lambda\}_{\lambda \in \mathbb{R}}$  que satisface

- $E_\lambda E_\mu = E_{\min\{\lambda, \mu\}}$
- Continua por la derecha
- $\lim_{\lambda \rightarrow -\infty} E_\lambda = 0$  y  $\lim_{\lambda \rightarrow \infty} E_\lambda = 1$

Una familia espectral define una medida espectral  $E$ , esto es una medida a valores proyecciones mediante  $E((a, b]) := E_b - E_a$ .

# Cálculo funcional para operadores autoadjuntos

## Teorema 2

*Dado un operador  $(A, D(A))$  autoadjunto. A toda función  $\varphi$  continua y acotada sobre  $\sigma(A)$  le corresponde un operador  $\varphi(A)$  definido por*

$$\varphi(A) = \int_{\sigma(A)} \varphi(\lambda) E(d\lambda) . \quad (17)$$

Además, si consideramos la estructura de  $C^*$ -álgebra en  $C_b(\sigma(A))$  (multiplicación puntual, conjugación compleja y norma del supremo) tenemos que  $\varphi \rightarrow \varphi(A)$  es un morfismo de  $C^*$ -álgebras y en particular es contractivo. Es decir:

$$\|\varphi(A)\| \leq \|\varphi\|_\infty . \quad (18)$$

## Tipos de espectro

A partir de la medida espectral, y para cada  $f \in \mathcal{H}$ , definimos una medida por  $m_f(O) = \|E(O)f\|^2$ . De aquí podemos deducir una descomposición de  $\mathcal{H}$

$$\mathcal{H} = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} \oplus \mathcal{H}_p .$$

tal que si  $f \in \mathcal{H}_{ac}$ , la medida  $m_f$  es absolutamente continua con respecto a la medida de Lebesgue. Análogamente se define la parte singular continua  $\mathcal{H}_{sc}$  y la parte puntual  $\mathcal{H}_p$ . En particular, si  $f$  es un vector propio, entonces  $f \in \mathcal{H}_p$ .



# Observables cuánticos

Un sistema cuántico está descrito por un vector (unitario) de un espacio de Hilbert. Un observable cuántico es un operador autoadjunto  $A$ . El espectro  $\sigma(A)$  son los valores posibles que puede tomar el observable  $A$ . Si  $E$  es la medida espectral asociada a  $A$ ,  $\varphi$  es el estado del sistema y  $O$  es un conjunto medible, la probabilidad de que el observable  $A$  exhiba un valor en  $O$  es

$$\|(\int_O E(d\lambda))\psi\|^2. \quad (19)$$

## Ejemplo 2

*En  $L^2(\mathbb{R})$  los dos principales observables que necesitamos son el operador posición  $(Q\varphi)(x) = x\varphi(x)$  y el observable momentum  $(-i\partial_x\varphi)(x) = -i\varphi'(x)$ . Son la cuantización los observables clásicos posición y momentum.*

# Relación entre observables clásicos y cuánticos

El movimiento de una partícula clásica está descrito por una curva  $t \rightarrow (x(t), \xi(t)) \in \mathbb{R}^3 \times \mathbb{R}^3$ . La energía total está dada

$$E = \frac{1}{2m} \xi(t)^2 + V(x(t)) . \quad (20)$$

Pasando al lado cuántico,  $E$  corresponde al operador de Schrödinger

$$H = -\frac{\hbar}{2m} \Delta + V(x) . \quad (21)$$

Un observable clásico es una función infinitamente diferenciable sobre el espacio de fase  $\mathbb{R}^3 \times \mathbb{R}^3$ . Dado un observable clásico  $a(x, \xi)$ , ¿cómo le podemos asignar un observable cuántico?

# Operadores pseudodiferenciales

Sea  $a$  un símbolo clásico. Formalmente definimos  $a^w(x, hD) = \text{Op}_h^w(a)$  por la siguiente fórmula donde  $u$  es un vector adecuado de  $L^2(\mathbb{R}^3)$

$$[\text{Op}_h^w(a)u](x) = \frac{1}{(2\pi h)^3} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} e^{\frac{i}{h}(x-y) \cdot \xi} a\left(\frac{x+y}{2}, \xi\right) dy d\xi. \quad (22)$$

## Ejemplo 3

Si  $a(x, \xi) = \sum_{|\alpha| \leq m} b_\alpha(x) \xi^\alpha$  entonces

$$\text{Op}_h^w\left(\sum_{|\alpha| \leq m} b_\alpha(x) \xi^\alpha\right) = \sum_{|\alpha| \leq m} (hD)^\alpha b_\alpha(x) \quad (23)$$

es un operador diferencial de orden  $m$ .

# Espacio de simbolos

Dado  $x \in \mathbb{R}^n$  definimos el corchete japonés por  $\langle x \rangle = (1 + x^2)^{\frac{1}{2}}$ .

## Definición 12

Decimos que  $m : \mathbb{R}^n \rightarrow \mathbb{R}_+$  es una función de orden si existen constantes  $C_0 > 0$  y  $N_0$  tales que  $m(x) \leq \langle x - y \rangle_0^{N_0} m(y)$

## Definición 13

$S(\mathbb{R}^n, m) = S(m)$  es el espacio de funciones  $a \in C^\infty(\mathbb{R}^n)$  talque para todo  $\alpha \in \mathbb{N}^n$ , existe  $C_\alpha > 0$  talque

$$|\partial^\alpha a(x)| \leq C_\alpha m(x) . \quad (24)$$

Decimos que  $\sum_j a_j h^j$  converge en el límite semiclásico a un simbolo  $a$  si  $a - \sum_{j=1}^N a_j h^j$  es de la forma  $h^{N+1} S(m)$  para todo  $N$ .

# Introducción al análisis semiclásico

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# Plan

- 1. Introduction : classical mechanics, quantum mechanics and semiclassical mechanics**
- 2. The functional calculus of  $h$ -pseudodifferential operators via the Helffer-Sjöstrand formula**
- 3. Trace formula for  $h$ -pseudodifferential operators**
- 4. Semiclassical Weyl's law**
- 5. Potential wells in 1D**

The initial goal of **semiclassical analysis** is to explore a central problem in physics which is the study of the relationship between **classical mechanics** and **quantum mechanics**. The starting point is the following famous principle :

**Bohr's correspondence principle (1923)** : One should recover the classical mechanics from the quantum mechanics when the Planck constant  $\hbar$  becomes negligible. In other words, classical mechanics is the limit of quantum mechanics when Planck's constant tends to zero.

## Classical mechanics

We start from a  $C^\infty$  function on  $\mathbb{R}^{2d}$  :  $(x, \xi) \mapsto p(x, \xi)$  which will permit to describe the motion of the system in consideration and is called the **classical Hamiltonian**. The variable  $x$  corresponds in the simplest case to the **position** and  $\xi$  to the **impulsion** of one particle. The evolution is then described, starting from a given point  $(y, \eta)$ , by the so called **Hamiltonian equations**

$$\frac{d}{dt}x(t) = \partial_\xi p(x(t), \xi(t)), \quad \frac{d}{dt}\xi(t) = -\partial_x p(x(t), \xi(t)), \quad (x(t), \xi(t))|_{t=0} = (y, \eta) \in \mathbb{R}^{2d}.$$

The **classical trajectories** are then defined as the integral curves of a vector field defined on  $\mathbb{R}^{2d}$  called the hamiltonian vector field associated with  $p$  and defined by  $H_p = (\partial_\xi p, -\partial_x p)$  :

$$\exp(tH_p)(y, \eta) = (x(t), \xi(t)) : \text{hamiltonian flow} \quad (t \in \mathbb{R}).$$

The time evolution of a classical observable  $q \in C^\infty(\mathbb{R}^{2d}; \mathbb{R})$  given by  $q_0(t, x, \xi) = q(\exp(tH_p)(x, \xi))$ ,  $t \in \mathbb{R}$ ,  $(x, \xi) \in \mathbb{R}^{2d}$ , is described by the equation

$$\frac{d}{dt}q_0(t, x, \xi) = \{p, q\}(\exp(tH_p)(x, \xi)), \quad q_0(t, x, \xi)|_{t=0} = q(x, \xi) \quad (1)$$

where  $\{p, q\} := \partial_\xi p \cdot \partial_x q - \partial_x p \cdot \partial_\xi q$  is the Poisson bracket of  $p, q$ .

In the framework of the classical mechanics the main questions could be :

- ▶ Are the trajectories bounded ?
- ▶ Are there periodic trajectories ?
- ▶ Is the energy surface compact ?

The solutions of the above questions could be very difficult. Let us just recall the **conservation of energy law**

$$\rho(\exp(tH_p)(x, \xi)) = \rho(x, \xi).$$

This means that for any energy  $E \in \mathbb{R}$ , the energy surface  $\rho^{-1}(E) = \{(x, \xi) \in \mathbb{R}^{2d}; \rho(x, \xi) = E\}$  is stable by the hamiltonian flow  $\exp(tH_p)$ .

## Quantum mechanics

The quantum theory is born around 1920. In quantum mechanics, our basic object will be a (possibly non-bounded) self-adjoint operator defined on a dense subspace of an Hilbert space  $\mathcal{H}$ . In order to simplify we shall always take  $\mathcal{H} = L^2(\mathbb{R}^d)$ .

This operator (quantum hamiltonian) can be associated with a symbol (classical hamiltonian)  $\rho$  by different techniques called quantizations. For instance one can work with the Weyl quantization :

$$C^\infty(\mathbb{R}^{2d}; \mathbb{R}) \ni \rho \longmapsto \text{Op}_h^W(\rho) \text{ a self-adjoint operator in } L^2(\mathbb{R}^d).$$

The operator  $P = \text{Op}_h^W(\rho)$  is called  **$h$ -pseudodifferential operator** of symbol  $\rho$ . Here  $h > 0$  is a small parameter which plays the role of the Planck constant called **the semiclassical parameter**.

Given such an operator, the dynamics of the quantum system is governed by the **Schrödinger equation**

$$ih \frac{d}{dt} \psi(t) = P\psi(t), \quad \psi(t)|_{t=0} = \psi_0 \in L^2(\mathbb{R}^d).$$

This equation generates a unitary operator called the evolution operator (or the propagator)  $e^{-\frac{it}{h}P}$  :

$$\psi(t) = e^{-\frac{it}{h}P} \psi_0 \quad (t \in \mathbb{R}).$$

The evolution in time of a quantum observable  $\text{Op}_h^W(q)$  given by

$$Q(t) := e^{\frac{it}{h}P} \text{Op}_h^W(q) e^{-\frac{it}{h}P}$$

is then described by the quantum analogous of equation (1) the so called **Heisenberg equation**

$$\frac{d}{dt} Q(t) = \frac{i}{h} [P, Q(t)], \quad Q(t)|_{t=0} = \text{Op}_h^W(q).$$



## Semiclassical mechanics

A rigorous mathematical justification of the correspondence principle is given by the following theorem known as **Egorov's theorem** :

$$Q(t) = \text{Op}_\hbar^W(q(\exp(tH_p))) + \mathcal{O}_{\mathcal{L}(L^2)}(\hbar)$$

uniformly for  $|t| \leq T$ , for all  $T \in \mathbb{R}$ . This result of course needs appropriate assumptions on the symbols  $p$  and  $q$ .

Semiclassical analysis is thus an asymptotic analysis which allows to establish the relation between quantum objects and classical objects in the **semiclassical limit**  $\hbar \rightarrow 0^+$  :

**Quantum objects** : quantum Hamiltonians (operators), eigenvalues, eigenfunctions, quantum resonances, resonance states, etc

Corresp. in the  
semiclassical limit  $\rightarrow$

**Classical objects** : classical hamiltonians (functions), volumes in the phase space, closed trajectories of the hamiltonian flow, Maslov's index, etc

To establish this correspondance, we often use techniques from **microlocal analysis**, **pseudodifferential calculus**, **Fourier Integral operators**, **symplectic geometry**, etc. The techniques of semiclassical analysis have found many applications in several fields where a small parameter appears naturally and plays an important role, for instance :

- The square root of the quotient between the electronic and nuclear masses in the Born-Oppenheimer approximation in **molecular dynamics**.
- The adiabatic parameter in **adiabatic theory**.
- The inverse of the square root of the position in **spectral problems in high-energy regime**.
- The inverse of the norm of the position in **scattering theory**.
- The inverse of the temperature in the study of the **metastability** (Langevin equation).

A prototype result in semiclassical analysis has the following form : Given a pseudodifferential operator  $\text{Op}_\hbar^W(p)$  with a symbol  $p$  defined on  $\mathbb{R}^{2d}$  and denoting  $H_p$  the corresponding hamiltonian field, under some reasonable assumptions on the symbol  $p$ , we have, in the semiclassical limit  $\hbar \rightarrow 0^+$ ,

A geometric property of the hamiltonian field  $H_p$

$\Rightarrow$

A spectral property of the operator  $\text{Op}_\hbar^W(p)$ .

In order to study the dynamical and spectral properties of  $h$ -pseudodifferential operators one needs to establish a **functional calculus** on these operators. **What is functional calculus?** Any formula which represents a function as a superposition of simpler functions can (at least in principle) be taken as a starting point for a functional calculus.

Recall that for a **self-adjoint operator**  $P$  on a Hilbert space  $\mathcal{H}$  and a "nice" **real-valued function**  $f$ , say a bounded continuous function, the spectral theorem allows us to define a **new linear bounded self-adjoint operator**  $f(P)$  as follows

$$f(P) = \int_{\mathbb{R}} f(t) dE_t$$

where  $E_t = 1_{(-\infty, t]}(P)$  is the family of spectral projections associated with  $P$ .

This formula is very useful in many problems in spectral theory. However, it is unfortunately a bit too abstract to work with! In particular, in the framework of semiclassical pseudodifferential operators, it is not convenient to answer the following natural questions :

- ▶ **Is  $f(P)$  a semiclassical pseudodifferential operator** if  $P$  is a semiclassical pseudodifferential operator and  $f$  is a "nice" function?
- ▶ If yes, do we have an **algorithm to compute the symbol of  $f(P)$**  from that of  $P$ ?
- ▶ If "yes and yes", is this formula good enough to use it in **the study of the spectral properties of the operator  $P$** ?

In the following we will introduce a formula for  $f(P)$  called the **Helffer-Sjöstrand formula** which allows us to answer the above questions. As we will see this formula is very useful in the spectral analysis of  $h$ -pseudodifferential operators since it relates  $f(P)$  with the resolvent  $(z - P)^{-1}$ .

## Almost analytic extensions

In all the talk  $C_0^\infty(\mathbb{R})$  stands for the space of  $C^\infty$  real-valued functions on  $\mathbb{R}$  with compact support.

For a function defined on  $\mathbb{C}$  (or  $\mathbb{R}^2$ ) we will use the operator

$$\bar{\partial} = \partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y).$$

We recall that if a function  $g$  is holomorphic on some open subset  $\Omega \subset \mathbb{C}$ , then  $\bar{\partial}g \equiv 0$  in  $\Omega$ .

**Definition.** Let  $f \in C_0^\infty(\mathbb{R})$ . We call **almost analytic extension** of  $f$  any function  $\tilde{f} \in C_0^\infty(\mathbb{C})$  satisfying

- 1)  $\tilde{f}|_{\mathbb{R}} = f$ .
- 2) For all  $N \in \mathbb{N}$ , there exists a constant  $C_N > 0$  such that

$$|\bar{\partial}^k \tilde{f}(z)| \leq C_N |\operatorname{Im} z|^N.$$

- ▶ The first condition just states that **the restriction of  $\tilde{f}$  on the real line coincides with  $f$** .
- ▶ The second condition is equivalent to the fact that  **$\bar{\partial}^k \tilde{f}$  vanishes at infinite order on the real line**, that is, if one identifies  $\mathbb{C} \ni z = x + iy \mapsto (x, y) \in \mathbb{R}^2$ :

$$\partial_y^k \bar{\partial} \tilde{f}(x, 0) = 0, \quad \forall k \in \mathbb{N}, x \in \mathbb{R}.$$

The notion of almost analytic extension was introduced by **Hörmander** in the 60's of the previous century and has subsequently been used by many people : **Nirenberg, Maslov, Kucherencko, Dynkin, Taylor**, etc.

## Almost analytic extensions

Given a function  $f \in C_0^\infty(\mathbb{R})$  there are many ways to construct an almost analytic extension  $\tilde{f} \in C_0^\infty(\mathbb{C})$  of  $f$ . A simple explicit way is given by the following proposition :

**Proposition.** Let  $f \in C_0^\infty(\mathbb{R})$ . Let  $\chi, \psi \in C_0^\infty(\mathbb{R})$  such that

$$\chi \equiv 1 \text{ near } 0, \quad \psi \equiv 1 \text{ near the support of } f.$$

Then

$$\tilde{f}(x + iy) = \frac{\psi(x)\chi(y)}{2\pi} \int_{\mathbb{R}} e^{i(x+iy)\xi} \chi(y\xi) \widehat{f}(\xi) d\xi$$

is an almost analytic extension of  $f$ . Here  $\widehat{f}(\xi) := \int_{\mathbb{R}} e^{-it\xi} f(t) dt$  stands for the Fourier transform of  $f$ .

**Proof.** The first property holds immediately by the Fourier inversion formula : we have for all  $x \in \mathbb{R}$

$$\tilde{f}(x + i0) = \frac{\psi(x)}{2\pi} \int_{\mathbb{R}} e^{ix\xi} \widehat{f}(\xi) d\xi = \psi(x)f(x) = f(x).$$

To prove the second property, notice that since  $x + iy \mapsto e^{x+iy\xi}$  is holomorphic,  $\bar{\partial}\tilde{f}$  is, up to the constant  $\frac{1}{4\pi}$ , the sum of the following three terms

$$I := \psi'(x)\chi(y) \int_{\mathbb{R}} e^{i(x+iy)\xi} \chi(y\xi) \widehat{f}(\xi) d\xi$$

$$II := i\psi(x)\chi'(y) \int_{\mathbb{R}} e^{i(x+iy)\xi} \chi(y\xi) \widehat{f}(\xi) d\xi$$

$$III := i\psi(x)\chi(y) \int_{\mathbb{R}} e^{i(x+iy)\xi} \chi'(y\xi) \xi \widehat{f}(\xi) d\xi$$

We have then to estimate each one of these terms.

## Almost analytic extensions

- In the first term  $I$ , we expand  $e^{-y\xi}\chi(y\xi)$  by the Taylor formula which gives a remainder of the form

$$\psi'(x)\chi(y) \int_{\mathbb{R}} e^{ix\xi} \mathcal{O}(|y\xi|^N) \widehat{f}(\xi) d\xi = \mathcal{O}(|y|^N)$$

and a linear combination of terms of the form

$$\psi'(x)\chi(y) \int_{\mathbb{R}} e^{ix\xi} (y\xi)^k \widehat{f}(\xi) d\xi = 0$$

since by the Fourier inversion formula, the integral equals  $y^k f^{(k)}(x)$  up to a multiplicative constant and since  $\psi'$  vanishes on the support of  $f$ .

- Obviously  $II$  vanishes near  $y = 0$ .
- In the last term  $III$ , using that  $\chi'$  vanishes near  $0$ , the integral can be written as

$$\int_{\mathbb{R}} e^{(x+iy)\xi} \frac{\chi'(y\xi)}{(y\xi)^N} y^N \xi^{N+1} \widehat{f}(\xi) d\xi = \mathcal{O}(|y|^N).$$

**Remark :** From the above construction we notice the following :

- ▶ An almost analytic extension is not unique.
- ▶ We can take  $\tilde{f}$  with support in an arbitrarily small neighborhood of the support of  $f$ .
- ▶ If  $g$  is the difference of two almost analytic extensions of the same function, so that  $g|_{\mathbb{R}} = 0$  and  $\bar{\partial}g = \mathcal{O}(|\text{Im } z|^N)$ , or all  $N \in \mathbb{N}$ , then  $g = \mathcal{O}(|\text{Im } z|^N)$  for all  $N \in \mathbb{N}$ .
- ▶ One can actually construct almost analytic extensions for a more general class of functions than  $C_0^\infty(\mathbb{R})$  (for instance Schwartz functions or even more general). But for our applications this class is sufficient.

## Integrals involving almost analytic extensions

For a continuous function  $B(x, y)$  defined on  $\mathbb{R}^2 \setminus \{y = 0\}$ , or equivalently on  $\mathbb{C} \setminus \mathbb{R}$ , with values in a Banach space, we shall denote

$$\int_{|\operatorname{Im} z| \geq \varepsilon} \bar{\partial} \tilde{f}(z) B(z) L(dz) := \int_{|y| \geq \varepsilon} \left( \int_{\mathbb{R}} \bar{\partial} \tilde{f}(x, y) B(x, y) dx \right) dy$$

and

$$\int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) B(z) L(dz) := \lim_{\varepsilon \rightarrow 0} \int_{|\operatorname{Im} z| \geq \varepsilon} \bar{\partial} \tilde{f}(z) B(z) L(dz).$$

The following result justifies the existence of integrals involving almost analytic extensions :

**Proposition.** Let  $f \in C_0^\infty(\mathbb{R})$  and  $\tilde{f}$  an almost analytic extension of  $f$  supported in  $[a, b] + i[c, d]$ . For all continuous function  $B : [a, b] + i[c, d] \setminus \mathbb{R} \rightarrow \mathfrak{B}$  with values in a Banach space  $\mathfrak{B}$  and such that, for some constants  $C, M > 0$ ,

$$\|B(z)\|_{\mathfrak{B}} \leq C |\operatorname{Im} z|^{-M}, \quad z \in [a, b] + i[c, d] \setminus \mathbb{R},$$

the following hold

- The integral

$$\int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) B(z) L(dz)$$

is well defined.

- We have the bound

$$\left\| \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) B(z) L(dz) \right\|_{\mathfrak{B}} \leq C \sup_{[a, b] + i[c, d] \setminus \mathbb{R}} \|(\operatorname{Im} z)^M B(z)\|_{\mathfrak{B}}.$$

**Proof.** By standard results, the map  $y \mapsto \int_{\mathbb{R}} \bar{\partial} \tilde{f}(x, y) B(x + iy) dx$  is continuous on  $[c, d] \setminus \{0\}$  and satisfies

$$\left\| \int_{\mathbb{R}} \bar{\partial} \tilde{f}(x, y) B(x + iy) dx \right\|_{\mathfrak{B}} \leq (b - a) \sup_{x \in [a, b]} \|y^M B(x + iy)\|_{\mathfrak{B}} \sup_{x \in [a, b]} \|y^{-M} \bar{\partial} \tilde{f}(x, y)\|_{\mathfrak{B}}$$

for all  $y \in [c, d] \setminus \{0\}$ . The result follows easily after an integration w.r.t.  $y$ .

# Helffer-Sjöstrand formula

**Theorem.** Let  $P$  be a self-adjoint operator on a Hilbert space  $\mathcal{H}$ . Let  $f \in C_0^\infty(\mathbb{R})$  and let  $\tilde{f} \in C_0^\infty(\mathbb{C})$  be an almost analytic extension of  $f$ . Then

$$f(P) = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) (z - P)^{-1} L(dz). \quad (2)$$

Before proving this result, let us first give some important remarks.

- Notice that the left hand side of (2) is well defined by the spectral theorem. For the right hand side, we recall that  $\|(z - P)^{-1}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(|\operatorname{Im} z|^{-1})$  for  $z \in \mathbb{C} \setminus \mathbb{R}$ , hence the integral is well defined according to the previous proposition.
- The right hand side of (2) doesn't depends on the particular choice of the almost analytic extension  $\tilde{f}$ : by Stoke's formula we have

$$I_{\tilde{f}} := \lim_{\varepsilon \rightarrow 0} -\frac{1}{\pi} \int_{|\operatorname{Im} z| > \varepsilon} \bar{\partial} \tilde{f}(z) (z - P)^{-1} L(dz) = \lim_{\varepsilon \rightarrow 0} \frac{i}{2\pi} \int_{\mathbb{R}} \left[ \tilde{f}(z) (z - P)^{-1} \right]_{z=t-i\varepsilon}^{z=t+i\varepsilon} dt.$$

- For any real number  $\lambda$  and any integer  $n \geq 0$ , one has the following Cauchy type formula

$$\frac{(-1)^n}{n!} f^{(n)}(\lambda) = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) (z - \lambda)^{-1-n} L(dz).$$

# Helffer-Sjöstrand formula

**Proof of the Theorem.** It suffices to apply the spectral theorem to both sides of the formula. More precisely, set

$$Q := -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) (z - P)^{-1} L(dz) \in \mathcal{L}(\mathcal{H}).$$

Let  $u, v \in \mathcal{H}$  and write

$$\langle (z - P)^{-1} u, v \rangle_{\mathcal{H}} = \int (z - t)^{-1} \langle dE_t u, v \rangle_{\mathcal{H}}$$

where  $E_t = 1_{(-\infty, t]}(P)$  is the family of spectral projections associated with  $P$ . Consequently,

$$\langle Qu, v \rangle_{\mathcal{H}} = -\frac{1}{\pi} \int \bar{\partial} \tilde{f}(z) \int (z - t)^{-1} \langle dE_t u, v \rangle_{\mathcal{H}} L(dz)$$

and by Fubini's theorem one gets

$$\begin{aligned} \langle Qu, v \rangle_{\mathcal{H}} &= \int \left( -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) (z - t)^{-1} L(dz) \right) \langle dE_t u, v \rangle_{\mathcal{H}} \\ &= \int f(t) \langle dE_t u, v \rangle_{\mathcal{H}} \\ &= \langle f(P)u, v \rangle_{\mathcal{H}}. \end{aligned}$$

This proves that  $Q = f(P)$ .



Using the Helffer-Sjöstrand formula we are now able to give an answer to the first question :

Is  $f(P)$  a semiclassical pseudodifferential operator if  $P$  is a semiclassical pseudodifferential operator and  $f$  is a "nice" function ?

Consider a **self-adjoint semiclassical pseudodifferential operator**  $P = \text{Op}_\hbar^w(p)$  defined on a dense subspace of a Hilbert space  $\mathcal{H}$ . In order to simplify we shall always take  $\mathcal{H} = L^2(\mathbb{R}^d)$ . The symbol of the operator  $P$  is a **smooth real-valued function**  $p : \mathbb{R}^{2d} \rightarrow \mathbb{R}$  which belongs to some class of symbols  $\mathcal{S}(m)$  for some order function  $m \geq 1$  :

$$|\partial_x^\alpha \partial_\xi^\beta p(x, \xi)| \leq C_{\alpha, \beta} m(x, \xi), \quad \forall \alpha, \beta \in \mathbb{N}^d, x \in \mathbb{R}^d.$$

The typical example is **the semiclassical Schrödinger operator**

$$P = -\hbar^2 \Delta + V(x)$$

where  $\Delta := \sum_{j=1}^d \partial_{x_j}^2$  is the Laplace operator in  $\mathbb{R}^d$  and  $V \in C^\infty(\mathbb{R}^d; \mathbb{R})$  is a smooth real-valued potential. The associated semiclassical symbol is given by  $p(x, \xi) = \xi^2 + V(x)$ ,  $(x, \xi) \in \mathbb{R}^{2d}$ .

We can keep in mind as guiding examples :

- $V \in C_0^\infty(\mathbb{R}^d; \mathbb{R})$ .
- The harmonic oscillator  $V(x) = \sum_{j=1}^d \mu_j x_j^2$ , with  $\mu_j > 0$ , which is the natural approximation of a potential near its minimum (when non-degenerate).
- $V \in C^\infty(\mathbb{R}^d; \mathbb{R})$  of long-range type :

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x \rangle^{-\delta - |\alpha|}, \quad \forall x \in \mathbb{R}^d, \alpha \in \mathbb{N}^d,$$

for some  $\delta > 0$ .

The following result is the main result of the functional calculus of semiclassical pseudodifferential operators. This result is due to **Helffer-Robert** (1983).

**Theorem.** Let  $f \in C_0^\infty(\mathbb{R})$ . Then  $f(P)$  is a semiclassical pseudodifferential operator with symbol in  $\mathcal{S}(m^{-k})$  for any  $k \in \mathbb{N}$ . More precisely, there exists a semiclassical symbol  $a = a(x, \xi; h) \in \cap_{k \in \mathbb{N}} \mathcal{S}(m^{-k})$  such that

$$f(P) = \text{Op}_h^w(a)$$

Moreover the symbol  $a$  admits the following asymptotic expansion in powers of  $h$

$$a(x, \xi; h) \sim \sum_{j \geq 0} h^j a_j(x, \xi) \quad \text{in } \mathcal{S}(m^{-1}) \quad (3)$$

with  $a_0(x, \xi) = f(p(x, \xi))$  and  $a_1(x, \xi) = 0$ .

Our objective now is to apply the functional calculus developed above to study the spectral properties of the operator  $P$ . Here we show an application for the study of the discrete spectrum.

## Counting function of eigenvalues

Consider a **self-adjoint** semiclassical pseudodifferential operator  $P(h) = \text{Op}_h^w(\rho)$  in  $L^2(\mathbb{R}^d)$  with real-valued symbol  $\rho$ . Let  $[a, b] \subset \mathbb{R}$  be an interval and assume that for  $h > 0$  small enough, the spectrum of  $P(h)$  near  $[a, b]$  is discrete :

$$\text{Spec}(P(h)) \cap [a - \eta, b + \eta] = \{\lambda_1(h) \leq \lambda_2(h) \leq \dots \leq \lambda_{N_h}(h)\}$$

for some  $\eta > 0$ , where each  $\lambda_j(h)$  is a discrete eigenvalue of  $P(h)$  of finite multiplicity.

As a consequence of the function calculus, this assumption is in general satisfied when  $\rho^{-1}([a - \eta, b + \eta]) \subset \mathbb{R}^{2d}$  is compact. For instance :

- $P(h) = -h^2\Delta + V(x)$  with  $V \in C^\infty(\mathbb{R}^{2d}; \mathbb{R})$  and  $V(x) \rightarrow 0$  as  $|x| \rightarrow +\infty$ . The spectrum of  $P(h)$  is discrete in any interval  $[a, b]$  with  $a < b < 0$ .
- The harmonic oscillator  $P(h) = -h^2\Delta + |x|^2$ . The spectrum of  $P$  is discrete in  $\mathbb{R}$ .

The **counting function of eigenvalues** of  $P(h)$  in  $[a, b]$  is defined by

$$N_h(P, [a, b]) := \#\{j, \lambda_j(h) \in [a, b]\}.$$

This is just the number of eigenvalues of  $P(h)$  in  $[a, b]$  counting multiplicities. Notice that

$$N_h(P, [a, b]) = \text{tr} [1_{[a, b]}(P(h))].$$

where  $1_{[a, b]}$  is the characteristic function of  $[a, b]$ .

**Theorem.** Suppose that  $p^{-1}([a - \eta, b + \eta]) \subset \mathbb{R}^{2d}$  is compact. Then for any  $f \in C_0^\infty([a, b])$ , the operator  $f(P)$  is a trace class operator on  $L^2(\mathbb{R}^d)$  and we have

$$\operatorname{tr} [f(P)] \sim (2\pi h)^{-d} \sum_{j=0}^{\infty} h^j \iint_{\mathbb{R}^{2d}} a_j(x, \xi) dx d\xi.$$

In particular

$$\operatorname{tr} [f(P)] = (2\pi h)^{-d} \iint_{\mathbb{R}^{2d}} f(p(x, \xi)) dx d\xi + \mathcal{O}(h^{-d+1}).$$

**Proof.** Let  $p_1$  be a real-valued symbol such that  $p_1(x, \xi) = p(x, \xi)$  for  $|(x, \xi)|$  large enough and  $\inf p_1 > b + \eta$ . Then

- 1)  $P$  and  $P_1 = \text{Op}_h^w(p_1)$  are essentially self-adjoint in  $L^2(\mathbb{R}^d)$  with the same domain.
- 2)  $\exists$  an open neighborhood  $\Omega$  of  $[a - \eta, b + \eta]$  such that  $(z - P_1)^{-1}$  is holomorphic for  $z \in \Omega$ .

Let  $f \in C_0^\infty(]a, b[)$  and let  $\tilde{f} \in C_0^\infty(\Omega)$  be an almost analytic extension of  $f$  such that  $\text{supp } \tilde{f} \subset \Omega$ . We have

$$f(P_1) = 0$$

since  $\text{Spec}(P_1) \cap I = \emptyset$ . For  $\text{Im } z \neq 0$ , we have the resolvent identity

$$(z - P)^{-1} = (z - P_1)^{-1} + (z - P)^{-1}(P - P_1)(z - P_1)^{-1}.$$

Putting this into the Helffer-Sjöstrand formula we get

$$\begin{aligned} f(P) &= -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) [(z - P_1)^{-1} + (z - P)^{-1}(P - P_1)(z - P_1)^{-1}] L(dz) \\ &= -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) [(z - P)^{-1}(P - P_1)(z - P_1)^{-1}] L(dz) \end{aligned}$$

Since  $p - p_1$  is compactly supported, the operator  $P - P_1$  is trace class with trace class norm  $\mathcal{O}(h^{-d})$  so we conclude that  $f(P)$  is of trace class and of trace class norm  $\mathcal{O}(h^{-d})$ .

To compute the trace, let  $\chi \in C_0^\infty(\mathbb{R}^{2d})$  be equal to 1 in a neighborhood of  $\text{supp } (p - p_1)$ . Then

$$f(P)(1 - \text{Op}_h^w(\chi)) = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z) [(z - P)^{-1}(P - P_1)(z - P_1)^{-1}(1 - \text{Op}_h^w(\chi))] L(dz)$$

and

$$\|f(P)(1 - \text{Op}_h^w(\chi))\|_{\text{tr}} = \mathcal{O}(h^N), \quad \forall N \in \mathbb{N}.$$

In particular for all  $N \in \mathbb{N}$

$$\text{tr}[f(P)] = \text{tr}[f(P)\text{Op}_h^w(\chi)] + \mathcal{O}(h^N)$$

We get the result from the previous results.

# Weyl's law

**Theorem.** Under the above assumptions, one has as  $h \rightarrow 0$

$$N_h(P, [a, b]) = \frac{1}{(2\pi h)^d} (\text{Vol}\{(x, \xi) \in \mathbb{R}^{2d}, p(x, \xi) \in [a, b]\} + o(1))$$

**Proof.** Pick two sequences of compactly supported smooth functions  $f_{1,\varepsilon}, f_{2,\varepsilon}$  that approaches the characteristic function  $1_{[a,b]}$  from below and from above

$$1_{[a+\varepsilon, b-\varepsilon]} \leq f_{1,\varepsilon} \leq 1_{[a,b]} \leq f_{2,\varepsilon} \leq 1_{[a-\varepsilon, b+\varepsilon]}$$

Then we have

$$\text{tr} [f_{1,\varepsilon}(P)] \leq \text{tr} [1_{[a,b]}] = N_h(P(h), [a, b]) \leq \text{tr} [f_{2,\varepsilon}(P)]$$

The conclusion follows from the trace formula of the above Theorem

$$\text{tr} [f_{j,\varepsilon}(P)] = (2\pi h)^{-d} \iint_{\mathbb{R}^{2d}} f_{j,\varepsilon}(p(x, \xi)) dx d\xi + \mathcal{O}(h^{-d+1})$$

by taking then limit  $\varepsilon \rightarrow 0$ .

## Example : The harmonic oscillator

Consider the  $d$ -dimensional harmonic oscillator

$$P(\hbar) = \frac{1}{2} (-\hbar^2 \Delta + |x|^2) = -\frac{\hbar^2}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} + \frac{|x|^2}{2}, \quad x \in \mathbb{R}^d.$$

We want to compute all the eigenvalues of  $P(\hbar)$ . To do so we introduce with the creation operators

$$C_k = \frac{1}{\sqrt{2}} \left( \frac{\hbar}{i} \frac{\partial}{\partial x_k} + ix_k \right)$$

and the annihilation operators

$$A_k = C_k^* = \frac{1}{\sqrt{2}} \left( \frac{\hbar}{i} \frac{\partial}{\partial x_k} - ix_k \right).$$

We have

$$[C_j, C_k] = 0 = [A_j, A_k] \quad \text{and} \quad [A_j, C_k] = \hbar \delta_{j,k} \cdot \text{Id}.$$

Moreover since

$$\begin{aligned} C_j A_j &= \frac{1}{2} \left( \frac{\hbar}{i} \frac{\partial}{\partial x_j} + ix_j \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x_j} - ix_j \right) \\ &= -\frac{\hbar^2}{2} \frac{\partial^2}{\partial x_j^2} + \frac{x_j^2}{2} - \frac{\hbar}{2} \end{aligned}$$

we get

$$P(\hbar) = \sum_{j=1}^d C_j A_j + \frac{d}{2} \hbar \cdot \text{Id} \tag{4}$$

and thus

$$[C_j, P(\hbar)] = -\hbar C_j \quad \text{and} \quad [A_j, P(\hbar)] = \hbar A_j.$$

It follows that if  $\lambda$  is an eigenvalue of  $P$ , that is  $Pu = \lambda u$ , then

$$PC_j u = [P, C_j]u + C_j Pu = hC_j u + C_j Pu = (\lambda + h)C_j u$$

and

$$PA_j u = (\lambda - h)A_j u.$$

This means that the creation operator  $C_j$  maps an eigenfunction  $u$  of  $P$  associated to the eigenvalue  $\lambda$  to an eigenfunction  $C_j u$  of  $P$  associated to the eigenvalue  $\lambda + h$ , while the annihilation operator  $A_j$  maps  $u$  to an eigenfunction  $A_j u$  (if it is nonzero) associated to the eigenvalue  $\lambda - h$ .

Observe from (4) that

$$\langle P(h)u, u \rangle = \sum_{j=1}^d \|A_j u\|^2 + \frac{d}{2} h \|u\|^2 \quad (5)$$

Then

- 1) If  $\lambda$  is an eigenvalue of  $P$  then  $\lambda \geq \frac{d}{2}h$ .
- 2) A function is an eigenfunction associated to  $\lambda = \frac{d}{2}h$  if and only if  $A_j u = 0$  holds for all  $1 \leq j \leq n$ .

A direct computation shows that

$$A_j u(x_j) = 0 \quad \Leftrightarrow \quad u(x_j) = ce^{-\frac{x_j^2}{2h}}.$$

and we see that  $\frac{d}{2}h$  is the smallest eigenvalue of  $P$  and the associated eigenfunction is  $u_0(x) = e^{-\frac{|x|^2}{2h}}$  which is often called **ground state**.

Starting from the ground state, one can find more eigenvalues using the creation operator : for any  $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ , the function

$$u_\alpha = C_1^{\alpha_1} \dots C_n^{\alpha_n} u_0$$

is an eigenfunction of  $P$  associated with the eigenvalue

$$\lambda_\alpha = \frac{d}{2}h + |\alpha|h.$$

Here  $|\alpha| = \sum_{j=1}^d \alpha_j$ .



The set  $\{\lambda_\alpha = \frac{d}{2}h + |\alpha|h\}$  contains all the eigenvalues of  $P(h)$ .

Indeed, if  $\lambda > \frac{d}{2}h$  is an eigenvalue of  $P$  with eigenfunction  $u$ , then by (5), there exists at least one  $j \in \{1, \dots, d\}$  such that  $A_j u \neq 0$ , and thus  $\lambda - h$  is also an eigenvalue of  $P$  with eigenfunction  $A_j u$ . As a consequence

- 1) Any eigenvalue of  $P$  with  $\lambda > \frac{d}{2}h$  must have the form  $\lambda = \frac{d}{2}h + kh$  for some  $k \in \mathbb{N}$ .
- 2) If  $u$  is the corresponding eigenfunction, then there exists  $\alpha_1, \dots, \alpha_n \in \mathbb{N}$  with  $|\alpha| = k$  such that  $A^\alpha u := A_1^{\alpha_1} \cdots A_n^{\alpha_n} u = u_0$ .

Finally, let us check Weyl's law for the harmonic oscillator. We have

$$\begin{aligned} \#\{j; \lambda_j \leq E\} &= \left\{ \alpha; \frac{d}{2}h + |\alpha|h \leq E \right\} \\ &= \left\{ \alpha; |\alpha| \leq \frac{1}{h} \left( E - \frac{d}{2}h \right) \right\} \\ &= \frac{1}{d!} \left( \frac{E}{h} \right)^d + o(h^{-d}) \end{aligned}$$

while

$$\text{Vol} \left\{ (x, \xi) \in \mathbb{R}^{2d}, \frac{1}{2} (|\xi|^2 + |x|^2) \leq E \right\} = (\sqrt{2E})^{2d} \times \text{the volume of the unit ball in } \mathbb{R}^{2d}.$$

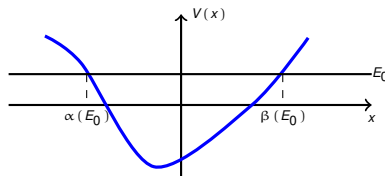
Weyl's law follows since the volume of the unit ball in  $\mathbb{R}^{2d}$  is  $\frac{\pi^d}{d!}$ .

Consider the semiclassical self-adjoint one-dimensional Schrödinger operator in  $L^2(\mathbb{R})$

$$P(\hbar) := -\hbar^2 \frac{d^2}{dx^2} + V(x)$$

with smooth real-valued potential  $V$  on the real line. Fix an energy-level  $E_0 \in \mathbb{R}$  and suppose that  $\liminf_{|x| \rightarrow +\infty} V(x) > E_0$  so that the spectrum of  $P(\hbar)$  consists of eigenvalues near  $E_0$ .

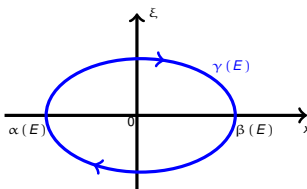
## Simple well



For  $E$  close to  $E_0$ , the corresponding energy surface (the characteristic set)

$$\gamma(E) := \left\{ (x, \xi) \in T^*\mathbb{R}; p(x, \xi) = E \right\}, \quad p(x, \xi) := \xi^2 + V(x)$$

is a smooth simple closed curve in the phase space  $T^*\mathbb{R} = \mathbb{R}_{x, \xi}^2$  symmetric w.r.t. the  $x$ -axis.



Here  $\alpha(E)$  and  $\beta(E)$  are the turning points, i.e. the zeros of  $V(x) - E$  near  $\alpha(E_0)$  and  $\beta(E_0)$  respectively.

**Action integral** : The action along the curve  $\gamma(E)$  is defined by the integral

$$\mathcal{A}(E) := \frac{1}{2} \int_{\gamma(E)} \xi dx = \int_{\alpha(E)}^{\beta(E)} \sqrt{E - V(x)} dx = \frac{1}{2} \int_{p(x, \xi) \leq E} dx d\xi.$$

**Bohr-Sommerfeld quantization rule.** The eigenvalues of  $P(\hbar)$  near  $E_0$  are approximated in the semiclassical limit  $\hbar \rightarrow 0^+$  by the roots of the equation

$$\cos\left(\frac{\mathcal{A}(E)}{\hbar}\right) = 0. \quad (\text{BS})$$

More precisely, we have

- 1) If  $E = E(\hbar)$  is an eigenvalue of  $P(\hbar)$  in a neighborhood of  $E_0$ , then there exists  $k = k(E; \hbar) \in \mathbb{N}$  such that

$$\mathcal{A}(E) = \left(k + \frac{1}{2}\right)\pi\hbar + \mathcal{O}(\hbar^2).$$

- 2) Conversely, for every  $k$  such that  $(k + \frac{1}{2})\pi\hbar$  belongs to a neighborhood of  $\mathcal{A}(E_0)$ , there exists an eigenvalue  $E_k(\hbar)$  of  $P(\hbar)$  satisfying

$$\left| \mathcal{A}(E_k(\hbar)) - \left(k + \frac{1}{2}\right)\pi\hbar \right| \leq C\hbar^2,$$

with a constant  $C > 0$  independent of  $k$  and  $\hbar$ .

### Remarks :

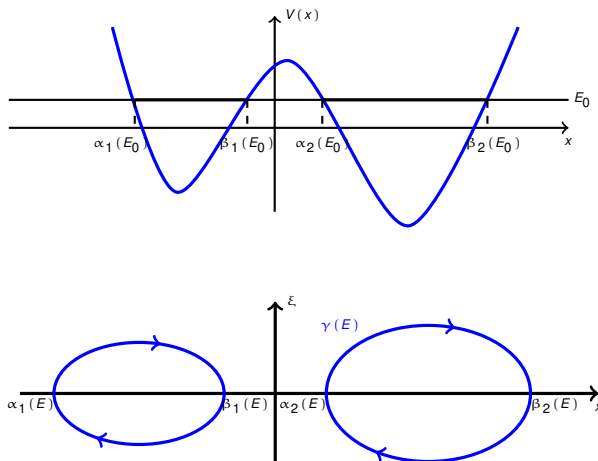
- There is exactly one eigenvalue of  $P(\hbar)$  in a neighb. of size  $\mathcal{O}(\hbar^2)$  of every root of (BS).
- The distance between two successive roots of (BS) is  $\sim \frac{\pi}{\mathcal{A}'(E_0)}\hbar$ .

$$\left[ \begin{array}{ccccccc} E_0 - \varepsilon & & & & & & E_0 + \varepsilon \\ & \times & \times & & \times & \times & \\ & & & & \underbrace{\times \times}_{\mathcal{O}(\hbar^2)} & \underbrace{\times \times}_{\mathcal{O}(\hbar^2)} & \end{array} \right] \quad \underbrace{\hspace{10em}}_{\mathcal{O}(\hbar)}$$

$\times$  = Roots of (BS);  $\times$  = Eigenvalues of  $P(\hbar)$

**Example :** **harmonic oscillator**  $V(x) = x^2$ . In this case  $\mathcal{A}(E) = \frac{\pi E}{2}$  and  $\sigma(P(\hbar)) = \left\{ (2k + 1)\hbar, k \in \mathbb{N} \right\}$ .

## Double well



The corresponding energy surface  $\gamma(E) := \{(x, \xi) \in T^*\mathbb{R}; \xi^2 + V(x) = E\}$  for  $E$  close to  $E_0$ .

**Theorem (Helffer-Sjöstrand '84)** The spectrum of  $P(h)$  near  $E_0$  is **exponentially close**, in the semiclassical limit  $h \rightarrow 0^+$ , to the union of the spectra of  $P$  restricted to each well :

$$\exists \text{ a bijection } b_h : \sigma(P) \text{ near } E_0 \rightarrow \bigcup_{j=1,2} \sigma(P|_{(\alpha_j, \beta_j)}) \text{ near } E_0$$

$$b_h(E) - E = \mathcal{O}(e^{-S(E)/h}) \text{ as } h \rightarrow 0^+,$$

where

$$S(E) := \int_{\beta_1(E)}^{\alpha_2(E)} \sqrt{V(x) - E} dx$$

is the so-called Agmon distance.

► **(BS) quantization rule for a simple well** : the eigenvalues of  $P_{|(\alpha_j, \beta_j)}$  near  $E_0$  are approximated in the semiclassical limit  $h \rightarrow 0^+$  by

$$\mathcal{U}_h^{(j)} := \left\{ E \text{ near } E_0; \cos \left( \frac{\mathcal{A}_j(E)}{h} \right) = 0 \right\} \quad (j = 1, 2)$$

where  $\mathcal{A}_j(E) := \int_{\alpha_j(E)}^{\beta_j(E)} \sqrt{E - V(x)} dx$  is the action associated with the well  $(\alpha_j(E), \beta_j(E))$ .

Assume that  $V$  is even (symmetric wells). In this case  $\mathcal{U}_h^{(1)} = \mathcal{U}_h^{(2)}$ .

► **LANDAU-LIFCHITZ '48** : Quantum tunneling effect between the two wells appears as eigenvalue splitting.

**Theorem (Gérard-Grigis '88)** The eigenvalues of  $P(h)$  near  $E_0$  come out in pairs with splitting exponentially small. If  $E_+(h)$  and  $E_-(h)$  are a pair of eigenvalues which are exponentially close to  $E \in \mathcal{U}_h^{(1)} \cup \mathcal{U}_h^{(2)}$ , then

$$|E_+(h) - E_-(h)| = \frac{2h}{\mathcal{A}'(E)} e^{-S(E)/h} + \mathcal{O}(e^{-2S(E)/h}) \quad (h \rightarrow 0^+)$$

where  $\mathcal{A}(E) := \mathcal{A}_1(E) = \mathcal{A}_2(E)$ .

**Remark** :  $\mathcal{A}'(E) = \frac{T(E)}{2}$  where  $T(E)$  is the period of the Hamiltonian flow  $(x(t), \xi(t))$  associated with the classical Hamiltonian  $\xi^2 + V(x)$ .