Semiclassical Dynamics
Master 2 course – ENS de Lyon

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(Version of March 13, 2025)

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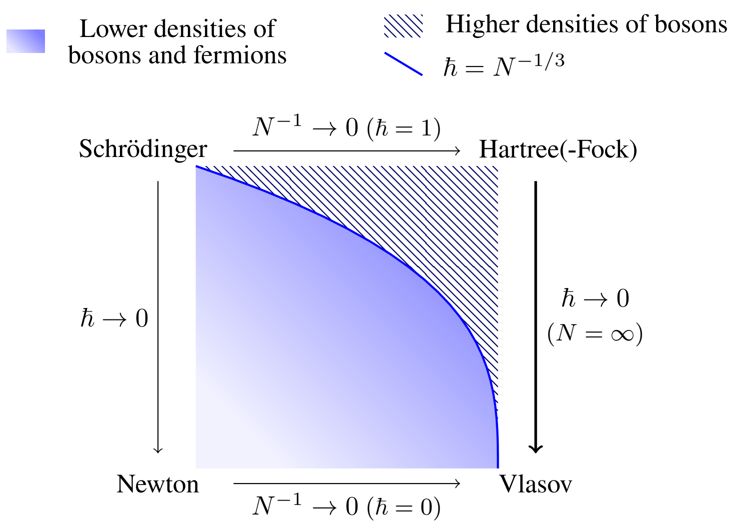
1 Introduction

1.1 Many body and semiclassical limits



1.2 Notation / Review of Functional Analysis

In all the course, we will work on functions from $\mathbb{R}^d$ to $\mathbb{C}$ (or as a special case $\mathbb{R}$), for some $d \in \mathbb{N}$ that can be thought to be either the dimension of the physical space $d = 3$, the dimension of a particular subsystem $d = 1$ or $d = 2$ or the dimension of some bigger system containing several particles or more complex generalizations.

1.2.1 Function spaces

Lebesgue spaces. In Lebesgue spaces, we will consider only functions in $L^1_{\text{loc}} = L^1_{\text{loc}}(\mathbb{R}^d, \mathbb{C})$, the set of locally integrable functions from $\mathbb{R}^d$ to $\mathbb{C}$, with the identifications of functions that are equal almost everywhere. The Lebesgue spaces L^p are then defined as the functions such that the norm

$$\|u\|_{L^p} := \left(\int_{\mathbb{R}^d} |u|^p\right)^{\frac{1}{p}} \text{ if } p \in [1, \infty)$$

is finite (or $\|u\|_{L^\infty} := \sup \operatorname{ess}_{\mathbb{R}^d} |u|$ when $p = \infty$). They are Banach spaces. If $(f, g) \in L^p \times L^{p'}$ with p' the Hölder conjugate[1] of p, we will denote by

$$\langle f, g \rangle = \int_{\mathbb{R}^d} f\, g \quad \text{and} \quad \langle f \,|\, g \rangle = \int_{\mathbb{R}^d} \overline{f}\, g.$$

Continuous functions C^n. The space of (possibly unbounded) continuous functions is denoted by

$$\dot{C}^0 := \{\, u : \mathbb{R}^d \to \mathbb{C} \mid \forall x \in \mathbb{R}^d, u(y) \underset{y \to x}{\to} u(x) \,\}$$

[1] $p' = \frac{p}{p-1}$ if $p \in (1, \infty)$, $p' = \infty$ if $p = 1$ and $p' = 1$ if $p = \infty$

while the space of bounded continuous functions is denoted by $C_b^0 := C^0 \cap L^\infty$. This latter space is a Banach space for the norm $\|u\|_{C_b^0} := \|u\|_{L^\infty}$. More generally, for $n \in \mathbb{N} = \{0, 1, 2, \dots\}$ we define the set of functions such that their n^{th} derivative is continuous by $\dot{C}^n = \{ u \in \dot{C}^0 \mid \nabla^n u \in \dot{C}^0 \}$ and by $C_b^n := \{ u \in C_b^0 \mid \nabla^n u \in C_b^0 \}$. It is a Banach space for the norm

$$\|u\|_{C_b^n} = \|u\|_{L^\infty} + \|\nabla^n u\|_{L^\infty} .$$

We define C_c^n as the set of functions in C^n that are compactly supported. In particular, C_c^∞ denotes the set of infinitely differentiable (smooth) compactly supported functions.

Sobolev spaces. Combining derivatives and Lebesgue spaces leads to the definition of the (inhomogeneous) Sobolev spaces $W^{n,p} := \{ u \in L^p, \nabla^n u \in L^p \}$, where the gradient is taken in the weak sense. They are Banach spaces for the norm

$$\|u\|_{W^{n,p}} := \|u\|_{L^p} + \|\nabla^n u\|_{L^p} .$$

We will also define the homogeneous Sobolev seminorms by $\|u\|_{\dot{W}^{n,p}} := \|\nabla^n u\|_{L^p}$. In the case $n = 2$ we write $H^n = W^{n,2}$.

We refer the reader not familiar with these notions to books such as [Bre83, LL01, AF03, Maz11, Tar07]

1.2.2 Distributions.

The purpose of the theory of distributions (created by L. Schwartz [Sch66]) is to provide a generalization of functions where all functions can be differentiated. The space of distributions $\mathcal{D}'$ is defined as the set of linear forms over the set[2] $\mathcal{D} = C_c^\infty$. For a distribution $f \in \mathcal{D}'$, we denote by

$$\langle f, \varphi \rangle_{\mathcal{D}',\mathcal{D}} := f(\varphi)$$

the action of f on a test function $\varphi \in \mathcal{D}$. Noticing that every $f \in L^1_{\text{loc}}$ defines a linear form given by $\varphi \mapsto \int_{\mathbb{R}^d} f\,\varphi$ and that this linear form characterizes completely f, we will identify functions $f \in L^1_{\text{loc}}$ with distributions by defining in this case

$$\langle f, \varphi \rangle_{\mathcal{D}',\mathcal{D}} := \int_{\mathbb{R}^d} f\,\varphi .$$

There are however other distributions that are not associated to any locally integrable function, such as the famous Dirac delta δ_0 defined by $\langle \delta_0, \varphi \rangle_{\mathcal{D}',\mathcal{D}} := \varphi(0)$. More generally, to every measure $\mu \in \mathcal{M}$, one can associate the distribution defined by $\langle \mu, \varphi \rangle_{\mathcal{D}',\mathcal{D}} := \int_{\mathbb{R}^d} \varphi(x)\,\mu(\mathrm{d}x)$, the integral of φ with respect to this measure. To generalize the notion of derivative, we define

$$\langle \nabla f, \varphi \rangle_{\mathcal{D}',\mathcal{D}} := - \langle f, \nabla \varphi \rangle_{\mathcal{D}',\mathcal{D}} ,$$

and this defines for every distribution f a new distribution ∇f. In the case when $f \in C^1_{\text{loc}}$, it corresponds to the usual gradient.

[2] The notation $\mathcal{D}$ is actually usually used because $\mathcal{D}$ is endowed with the topology requiring convergence on each $C^k(\Omega)$ for each $k \in \mathbb{N}$ and each compact $\Omega \subset \mathbb{R}^d$

1.2.3 Fourier transform.

If $f \in L^1$, we take the convention that its Fourier transform is defined by

$$\mathcal{F}(u)(x) = \widehat{u}(x) = \int_{\mathbb{R}^d} e^{-2i\pi\, x\cdot y}\, u(y)\,\mathrm{d}y\,.$$

More generally, for any tempered distributions $f \in \mathcal{S}'$, where $\mathcal{S}$ denotes the dual of the Schwartz space $\mathcal{S}$, one defines the Fourier transform by the formula

$$\left\langle \widehat{f}, \varphi \right\rangle_{\mathcal{S}',\mathcal{S}} := \langle f, \widehat{\varphi}\rangle_{\mathcal{S}',\mathcal{S}}\,.$$

With this convention, the Fourier transform satisfies the following relations.

- ***Fourier inversion theorem:*** $\mathcal{F}^{-1}(u) = \widehat{u}(-x)$ (or equivalently $\widehat{\widehat{u}}(x) = u(-x)$.
- ***Affine transformations:*** $\widehat{u(\lambda\, y)} = \frac{1}{|\lambda|^d}\,\widehat{u}(x/\lambda)$ and $\mathcal{F}(u(x+a)) = e^{2i\pi\, x\cdot a}\,\widehat{u}(x)$
- ***Product and convolution:*** $\mathcal{F}(u * v) = \widehat{u}\,\widehat{v}$ and $\widehat{u\,v} = \widehat{u} * \widehat{v}$.
- ***Derivatives:*** $\mathcal{F}(\nabla u) = 2i\pi\, x\,\widehat{u}(x)$, or equivalently[3], $\mathcal{F}(x\,u(x)) = \frac{i}{2\pi}\nabla\widehat{u}$
- ***Integral:*** If $u \in L^1$, $\widehat{u}(0) = \int_{\mathbb{R}^d} u$ or if $\widehat{u} \in L^1$, $\int_{\mathbb{R}^d}\widehat{u} = u(0)$
- ***Scalar product:*** $\langle \widehat{u}, v\rangle = \langle u, \widehat{v}\rangle$ and $\langle \widehat{u}\,|\,v\rangle = \langle u\,|\,\widehat{v}\rangle$.

This last property implies that the Fourier transform is an isometry on L^2. On other Lebesgue spaces, we have the Hausdorff–Young's inequality (see e.g. [LL01]), which tells that if $p \in [1,2]$ and $q = p'$, then

$$\|\widehat{u}\|_{L^q} \leq \left(\frac{p^{1/p}}{q^{1/q}}\right)^{d/2} \|u\|_{L^p}\,.$$

Bounds on L^q norms of the Fourier transform with $p < 2$ cannot be obtained with the only information that $u \in L^p$. A sufficient condition[4] to have $\widehat{u} \in L^1$ is to have $u \in H^s$ with $s > d/2$.

A fundamental example of Fourier transform is the Fourier transform of a Gaussian

$$\mathcal{F}\left(e^{-\lambda\pi|y|^2}\right) = \frac{1}{\lambda^{d/2}}\, e^{-\pi|x|^2/\lambda}$$

if $\lambda \in \mathbb{C}$ and $\mathrm{Re}(\lambda) \geq 0$. In particular, $e^{-\pi|x|^2}$ is its own Fourier transform. Another example is the case of the function $K_\alpha(x) = \frac{1}{|x|^\alpha}$ with $\alpha \leq d$, for which[5]

$$\mathcal{F}\left(\frac{1}{\omega_\alpha\,|y|^\alpha}\right) = \frac{1}{\omega_{d-\alpha}\,|x|^{d-\alpha}}$$

[3] In particular, $\mathcal{F}(hx\,u(x)) = i\hbar\,\nabla\widehat{u}$ since $\hbar = h/(2\pi)$

[4] For people knowing Besov spaces, one has some slightly more precise embeddings

$$H^s \subset B^{d/2}_{2,1} \subset \dot{B}^{d/2}_{2,1} \subset \mathcal{F}\left(L^1\right) \subset B^0_{\infty,1} \subset C^0$$

[5] The formula remains true for $\alpha \in \mathbb{R} \setminus ((d+2\mathbb{N}) \cup (-2\mathbb{N}))$ with the correct interpretation of $|x|^{-\alpha}$ as a distribution, using the Hadamard finite part. In the other cases, some logarithm appear. For example, if $\alpha = d$ and one defines $\frac{1}{|x|^d} := \mathrm{div}\left(\frac{x\ln(|x|)}{|x|^d}\right)$ with the divergence taken in the sense of distributions, then it is a good exercise to prove that $\mathcal{F}\left(\frac{1}{\omega_d\,|y|^d}\right) = \frac{\psi^{(0)}(d/2)-\gamma}{2} - \ln(|\pi x|)$ with $\psi^{(0)} := \frac{\Gamma'}{\Gamma}$ the digamma function.

with[6] $\omega_d = \frac{2\,\pi^{d/2}}{\Gamma(d/2)}$. It explains in particular why the Coulomb potential, solution of the Poisson equation $-\Delta K = \rho$, or equivalently $4\pi^2 |y|^2 \widehat{K} = \widehat{\rho}$, is given by $K(x) = \frac{\omega_2}{4\pi^2 \omega_{d-2}} \frac{1}{|x|}$. Let us finally also mention that in dimension $d = 3$, the Yukawa potential, which appears in plasma physics as a screened Coulomb potential, gives the the integral kernel of the operator $\left(1 - \frac{\Delta}{2\pi}\right)^{-1}$ thanks to the Formula

$$\mathcal{F}\left(\frac{1}{1 + |y|^2}\right) = \frac{e^{-2\pi|x|}}{|x|}\,.$$

1.2.4 Operators

General definitions. We will denote by $\mathcal{L}(X, Y)$ the set of (possibly unbounded) linear operators A from some domain $D(A) \subseteq X$ to Y and by $\mathcal{L}^\infty(X, Y)$ the set of bounded operators from X to Y (i.e. continuous operators). We write $\mathcal{L}^\infty(X) = \mathcal{L}^\infty(X, X)$. The operator norm is defined by

$$\|A\|_{\mathcal{L}^\infty(X,Y)} := \sup_{\psi \in X \setminus \{0\}} \frac{\|A\psi\|_Y}{\|\psi\|_X} = \sup_{\|\psi\|_X \leq 1} \|A\psi\|_Y\,.$$

If $A \in \mathcal{L}^\infty(X, Y)$, then[7] $D(A) = X$.

The set of compact operators from X to Y will be denoted by $\mathcal{K}(X, Y)$ (again, $\mathcal{K}(X) = \mathcal{K}(X, X)$). It is a closed ideal of $\mathcal{L}^\infty(X, Y)$ and if X is an Hilbert space, then $\mathcal{K}(X)$ satisfies the approximation property: compact operators are the limit of finite rank operators in the operator norm. The set of isometries is the set $\mathcal{I}(X, Y) = \{\, U \in \mathcal{L}(X, Y), \|Ux\|_Y = \|x\|_X \,\}$.

Hilbert space setting. Let $\mathcal{H}$ be a complex separable Hilbert space. In general we will look at $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C})$ with scalar product

$$\langle \varphi \,|\, \phi \rangle = \int_{\mathbb{R}^d} \overline{\varphi}\, \phi\,.$$

We will denote by $\mathcal{K} := \mathcal{K}(\mathcal{H})$ and $\mathcal{L}^\infty := \mathcal{L}^\infty(\mathcal{H})$ with the norm

$$\|A\|_\infty = \|A\|_{\mathcal{L}^\infty(\mathcal{H})}\,.$$

If $A \in \mathcal{L}(\mathcal{H})$, then its **adjoint** A^* is the operator with domain

$$D(A^*) = \{\, \varphi \in \mathcal{H} : \exists \psi \in H, \forall \phi \in H, \langle \varphi \,|\, A\phi \rangle = \langle \psi \,|\, \varphi \rangle \,\}$$

satisfying

$$\langle \varphi \,|\, A\phi \rangle = \langle A^* \varphi \,|\, \phi \rangle\,.$$

and an operator is said to be **self-adjoint** iff $A^* = A$ (in particular, it implies $D(A) = D(A^*)$) and **positive** iff $\forall \varphi \in D(A), \langle \varphi \,|\, A\varphi \rangle \geq 0$. We then write $A \geq 0$. More generally, we will write $A \leq B$ if $B - A \geq 0$. Self-adjoint operators can be seen as the analogue of real numbers among complex numbers. For instance, bounded positive operators are self-adjoint. Notice also that

$$\langle \psi \,|\, A\psi \rangle = \overline{\langle A\psi \,|\, \psi \rangle} = \overline{\langle \psi \,|\, A^*\psi \rangle} = \overline{\langle \psi \,|\, A\psi \rangle} \in \mathbb{R}\,.$$

[6]This is the volume of the unit sphere of $\mathbb{R}^d$ when $d \in \mathbb{N}$

[7]This is not true in general in $\mathcal{L}(X, Y)$. Think for instance to the Laplacian operator, defined on $H^2 \subset L^2$.

We also define $|A| = \sqrt{A^*A}$ as the positive operator such that $|A|^2 = A^*A$. Notice that isometries preserve the scalar product (i.e. $\langle U\phi \,|\, U\varphi\rangle_{\mathcal{H}} = \langle \phi \,|\, \varphi\rangle_{\mathcal{H}}$) and so $\mathcal{I} := \mathcal{I}(\mathcal{H}) = \{ U \in \mathcal{L}^\infty, |U| = 1 \}$. Finally, the set $\mathcal{U}$ of **unitary** operators is defined as the set of invertible isometries, that is

$$\mathcal{U} := \{ U \in \mathcal{I}, U \text{ is invertible} \} = \{ U \in \mathcal{L}^\infty, |U| = |U^*| = 1 \} .$$

It follows that $U^{-1} = U^* \in \mathcal{U}$.

Examples:

- Multiplication by a complex number of norm 1.
- Dilatation: let $a > 0$ and $\mathsf{h}_a\varphi(x) = a^{d/2}\varphi(a\,x)$. Then $\|\mathsf{h}_a\varphi\|_{L^2} = \|\varphi\|_{L^2}$ and $\mathsf{h}_a^{-1} = \mathsf{h}_{a^{-1}}$, so $\mathsf{h}_a \in \mathcal{U}$.

Spectrum. The spectrum of an operator $A \in \mathcal{L}(\mathcal{H})$ is defined by

$$\sigma(A) := \{ \lambda \in \mathbb{C}, \lambda - A \text{ is not invertible} \}$$

where $\lambda = \lambda \operatorname{Id}_{\mathcal{H}}$. If A is bounded, then $\sigma(A)$ is a compact set and $\sigma(A) \subseteq \bar{B}(0, \|A\|_\infty)$. The point spectrum is the set of eigenvalues, that is

$$\sigma_p(A) = \{ \lambda \in \mathbb{C}, \lambda - A \text{ is not injective} \} = \{ \text{eigenvalues} \} .$$

If $\mathcal{H}$ is finite dimensional, $\sigma(A) = \sigma_p(A)$. The diagonalization of symmetric matrices as the following counterpart for compact operators.

Theorem 1.1 (Spectral theorem for compact self-adjoint operators)**.** *Let $A \in \mathcal{K}$ be a self-adjoint operator. Then there exists a sequence of nonzero real numbers $(\lambda_j)_{j\in J}$ finite or converging to 0 and an Hilbert basis $(\psi_j)_{j\in J} \cup (\psi_j)_{j\in\mathbb{N}\setminus J}$ such that*

- $\sigma(A) = (\lambda_j)_{j\in J} \cup \{ 0 \}$,
- $(\psi_j)_{j\in\mathbb{N}\setminus J}$ *is a basis of* $\operatorname{Ker}(A)$,
- $\forall j \in J, A\,\psi_j = \lambda_j\,\psi_j$,
- $\forall \lambda \in \sigma(A) \setminus \{ 0 \}, \operatorname{Ker}(\lambda - A)$ *is finite dimensional.*

Remark 1.2.1. Notice that A can still be injective, in which case $0 \in \sigma(A) \setminus \sigma_p(A)$.

Remark 1.2.2. If $A \geq 0$, then the eigenvalues λ_j are also positive.

We will be using Dirac's bra-ket notation. If $\psi \in \mathcal{H}$, then $|\psi\rangle$ and $\langle\psi|$ defined by

$$|\psi\rangle = \psi \qquad\qquad \langle\psi|\,\varphi = \langle\psi\,|\,\varphi\rangle$$

are, respectively, the bra and ket of ψ, so that $|\psi\rangle\,\langle\psi|$ is the operator defined by

$$|\psi\rangle\,\langle\psi|\,\varphi(x) = \psi(x)\,\langle\psi\,|\,\varphi\rangle = \psi(x)\int_{\mathbb{R}^d} \overline{\psi(y)}\,\varphi(y)\,\mathrm{d}y\,.$$

By the above theorem, compact self-adjoint operators can be written

$$A = \sum_{j\in J} \lambda_j\,|\psi_j\rangle\,\langle\psi_j|\,. \tag{1}$$

In particular, the functional calculus tells us that we can define the function of an operator, which in this case can be defined by the formula

$$g(A) = \sum_{j\in J} g(\lambda_j) \left|\psi_j\right\rangle \left\langle\psi_j\right| .$$

The fact that ψ_j is an Hilbert basis gives that

$$\mathrm{Id}_{\mathcal{H}} = \sum_{j\in\mathbb{N}} \left|\psi_j\right\rangle \left\langle\psi_j\right| .$$

Trace of operators. For a compact operator A, one can define the trace when it exists (we will see later in more details) by the formula

$$\mathrm{Tr}(A) = \sum_{k\in\mathbb{N}} \langle \phi_k \mid A\phi_k \rangle \tag{2}$$

where $(\phi_k)_{k\in\mathbb{N}}$ is an orthonormal basis. It does not depend on the basis. In the particular case of self-adjoint compact operators of the form (1), taking $\phi_k = \psi_k$ yields

$$\mathrm{Tr}(A) = \sum_{j\in J} \lambda_j .$$

Hilbert–Schmidt operators. The Hilbert–Schmidt norm is defined by

$$\|A\|_2^2 = \sum_{k\in\mathbb{N}} \|A\phi_k\|_{L^2}^2 \tag{3}$$

where $(\phi_k)_{k\in\mathbb{N}}$ is an orthonormal basis. Notice that

$$\|A\|_2^2 = \sum_{k\in\mathbb{N}} \langle A\phi_k \mid A\phi_k \rangle = \sum_{k\in\mathbb{N}} \langle \phi_k \mid A^*A\phi_k \rangle = \mathrm{Tr}\Big(|A|^2\Big) .$$

In particular, it does not depend on the basis. In the particular case of self-adjoint compact operators of the form (1), the Hilbert–Schmidt norm is simply given by

$$\|A\|_2^2 = \sum_{j\in J} \lambda_j^2 .$$

If $K \in L^2(\mathbb{R}^{2d})$, then the integral operator given by

$$K\varphi(x) = \int_{\mathbb{R}^d} K(x,y)\,\varphi(y)\,\mathrm{d}y$$

is called an **Hilbert–Schmidt integral operator**. By the Cauchy–Schwarz inequality, it is bounded and $\|K\|_\infty \leq \|K\|_{L^2(\mathbb{R}^{2d})}$. By abuse of notation, we use the same letter for the operator K and its integral kernel. Notice that taking the adjoint yields

$$K^*(x,y) = \overline{K(y,x)} .$$

Sometimes, in analogy with matrices, one defines the transpose $K^\top(x,y) = K(y,x)$. Then the adjoint is the transpose-conjugate $K^* = \overline{K}^\top$.

Proposition 1.2. *Hilbert–Schmidt integral operators are compact Hilbert–Schmidt operators satisfying*

$$\|K\|_2 = \|K\|_{L^2(\mathbb{R}^{2d})} \,.$$

Proof. Let ϕ_j be an Hilbert basis of $\mathcal{H} = L^2(\mathbb{R}^d)$. Then $\overline{\phi_j} \otimes \phi_k$ is a basis of $\mathcal{H} \otimes \mathcal{H} = L^2(\mathbb{R}^{2d})$. Let $\psi_j := K\,\phi_j$ and

$$c_{k,j} = \langle \phi_k \,|\, K\phi_j \rangle = \langle \phi_k \,|\, \psi_j \rangle = \big\langle \overline{\phi_j} \otimes \phi_k \,\big|\, K \big\rangle_{L^2(\mathbb{R}^{2d})} \,.$$

Therefore, by the Parseval identity

$$\|K\|_2^2 = \sum_{j=1}^{\infty} \|\psi_j\|_{L^2}^2 = \sum_{j,k=1}^{\infty} |c_{k,j}|^2 = \|K\|_{L^2(\mathbb{R}^{2d})}^2 < \infty \,.$$

Now noticing that

$$K = \sum_{j=1}^{\infty} K\,|\phi_j\rangle\,\langle\phi_j| = \sum_{j=1}^{\infty} |\psi_j\rangle\,\langle\phi_j|$$

we can define the finite rank operator K_n by restricting the above sum to $j \in \{\,1,\ldots,n\,\}$. Then by the Cauchy–Schwarz inequality

$$\|(K - K_n)\varphi\|_{L^2}^2 \leq \left(\sum_{j=n+1}^{\infty} |\langle \phi_j \,|\, \varphi\rangle|^2\right) \sum_{j=n+1}^{\infty} \|\psi_j\|_{L^2} \leq \|\varphi\|_{L^2}^2 \sum_{j=n+1}^{\infty} \|\psi_j\|_{L^2}$$

and so $\|K - K_n\|_\infty \leq \left(\sum_{j=n+1}^{\infty} \|\psi_j\|_{L^2}\right)^{1/2} \to 0$, implying that K is compact as a limit of finite rank operators. □

Remark 1.2.3. If A is a self-adjoint compact Hilbert–Schmidt operator in the diagonal form (1), one gets that its integral kernel is given by

$$A(x,y) = \sum_{j\in J} \lambda_j\,\psi_j(x)\,\overline{\psi_j(y)}$$

and so, at least formally, its trace is given in terms of its kernel by

$$\mathrm{Tr}(A) = \sum_{j\in J} \lambda_j = \int_{\mathbb{R}^d} A(x,x)\,\mathrm{d}x \,.$$

One can associate integral kernels to more general operators thanks to the following theorem.

Theorem 1.3 (Schwartz kernel theorem)**.** *The operator $A \in \mathcal{L}^\infty(\mathcal{S},\mathcal{S}')$ iff there exists $A(\cdot,\cdot) \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ such that for any $(\varphi,\phi) \in \mathcal{S}(\mathbb{R}^d)^2$,*

$$\langle A\phi, \varphi\rangle_{\mathcal{S}',\mathcal{S}} = \langle A, \phi \otimes \varphi\rangle_{\mathcal{S}'(\mathbb{R}^d\times\mathbb{R}^d),\mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)}$$

which can be written more informally

$$A\phi(x) = \int_{\mathbb{R}^d} A(x,y)\,\phi(y)\,\mathrm{d}y \;\; \textit{in the sense of distributions.}$$

Let us give examples of generalized kernel:

$$\begin{array}{rcl}\mathrm{Id} & \longleftrightarrow & \delta_0(x-y)\\ \nabla & \longleftrightarrow & \nabla\delta_0(x-y)\\ \mathcal{F} & \longleftrightarrow & e^{-2i\pi\, x\cdot y}\\ (-\Delta)^{-1} & \longleftrightarrow & \dfrac{1}{4\pi\,|x-y|} \qquad\qquad \text{(in dimension } d=3)\end{array}$$

2 Classical and quantum mechanics

2.1 N interacting particles

We are interested in the case of N particles with positions x_1, ..., x_N, and velocities v_1, ..., v_N and, to simplify, with a common mass m. They can be thought of as microscopic particles such as electrons in a plasma, but could also correspond to stars in a galaxy. In the context of classical mechanics, the movement of these particles is given by Newton laws and leads to the following system of ordinary differential equations.

$$\begin{aligned}\dot{x}_k &= v_k\\ m\,\dot{v}_k &= F_k(x_1,\dots,x_N)\,.\end{aligned}$$

where the dot indicates the derivative with respect to time and F_k is the force applied to the k^{th} particle. The number of particles is however usually very large. A good example of the order of magnitude is given by the Avogadro number $N_A = 6.022\,140\,76 \times 10^{23}\,\mathrm{mol}^{-1}$. This prevents to perform exact numerical computations.

2.2 Kinetic Models

In the limit of a large number of particles, we want to simplify the N particle system by looking at the distribution of particles in the phase space $f(t,x,v)$, i.e. the number density of particles which are located at the position x and have velocity v at time t.

2.2.1 Averaged quantities

Using this distribution of particles, one can then express the typical observables of statistical mechanics. For example the proportion of particles with positions in Ω and velocity in $\mathcal{V}$ is given by

$$\iint_{\Omega\times\mathcal{V}} f(t,x,v)\,\mathrm{d}x\,\mathrm{d}v$$

and the total kinetic energy is given by

$$\mathcal{E}_c(t) = \frac{1}{2}\iint_{\mathbb{R}^{2d}} m\,|v|^2\, f(t,x,v)\,\mathrm{d}x\,\mathrm{d}v\,.$$

One can also consider local quantities defined at each point $x\in\mathbb{R}^d$ such as

- the (spatial) density of particles

$$\rho_f(t,x) = \int_{\mathbb{R}^d} f(t,x,v)\,\mathrm{d}v\,,$$

- the local mean velocity

$$u(t,x) = \frac{1}{\rho_f(t,x)} \int_{\mathbb{R}^d} f(t,x,v)\, v \,\mathrm{d}v\,,$$

- the temperature

$$\theta(t,x) = \frac{m}{3\,k_B\,\rho_f(t,x)} \int_{\mathbb{R}^d} f(t,x,v)\, |v-u|^2 \,\mathrm{d}v\,.$$

2.2.2 Volume preserving dynamics

We define the flow

$$Z : t \mapsto (X(t), V(t)) = (X(t,x_0,v_0), V(t,x_0,v_0))$$

solving to the Newton differential system of equations

$$\begin{aligned} \dot{X}(t) &= V(t) \\ m\,\dot{V}(t) &= F(t, X(t), V(t)) \end{aligned}$$

with initial conditions $(X(0,x_0,v_0), V(0,x_0,v_0)) = (x_0,v_0)$. For any $\Omega_0 \in \mathbb{R}^{2d}$, define $\Omega_t = \{\,(X(t),V(t))\,,(x_0,v_0) \in \Omega_0\,\}$. Then if there is no creation or destruction of particles and the flow is volume preserving,

$$\begin{aligned} \iint_{\Omega_{t_0}} f(t_0,x_0,v_0)\,\mathrm{d}x_0\,\mathrm{d}v_0 &= \iint_{\Omega_t} f(t,x,v)\,\mathrm{d}x\,\mathrm{d}v \\ &= \iint_{\Omega_{t_0}} f(t,X(t),V(t))\,\mathrm{d}x\,\mathrm{d}v\,. \end{aligned}$$

Since this holds for every $\Omega_0 \in \mathbb{R}^{2d}$, the number of particles does not change on the trajectories of the particles and so in the sense of measures

$$f(t, X(t), V(t)) = f(t_0, x_0, v_0)\,.$$

Therefore, taking the derivative with respect to time, we find the Liouville equation

$$\partial_t f + v \cdot \nabla_x f + \tfrac{F}{m} \cdot \nabla_v f = 0 \tag{4}$$

also called the Vlasov equation when the force depends on f.

Hamiltonian system case. In the case when the force is derived from a potential, then $F = -\nabla U$ and one can write the Vlasov equation as

$$\partial_t f = \{H, f\} \tag{5}$$

where the Hamiltonian is given by

$$H = \frac{|p|^2}{2\,m} + U \tag{6}$$

with $p = m\,v$ and the Poisson brackets are defined by $\{g,f\} = \nabla_x g \cdot \nabla_p f - \nabla_p g \cdot \nabla_x f$. In the case of a pair interaction $K(x,y)$, the mean-field model consist in assuming that the potential (or the force) at a point x is given by the average over all the other points y of the potential due to the point y, and so the mean-field potential is given by

$$U(x) = \int_{\mathbb{R}^d} K(x,y)\,\rho_f(y)\,\mathrm{d}y\,.$$

In the particular case where the pair interaction is translation invariant, we can write $K(x,y) = K(x-y)$ and then $U = K * \rho_f$. Since the force is independent of the velocity, integrating Equation (4) with respect to time yields the conservation of mass (or continuity equation)

$$\partial_t \rho_f + \operatorname{div} j = 0\,,$$

where the flux j is given by $j = \rho_f\, u$. The Hamiltonian system structure also leads to the conservation of the Lebesgue measure, as can be seen as writing Equation (4) in divergence form in the phase space and noticing that the flux is divergence free. This leads to the conservation of the so called Casimir invariants: for any function Φ, quantities of the form

$$\int_{\mathbb{R}^{2d}} \Phi(f)\,\mathrm{d}x\,\mathrm{d}v\,,$$

are conserved. Interesting examples are the Lebesgue norms $\|f\|_{L^p(\mathbb{R}^{2d})}$ with $p \in [0,\infty]$ or the entropy

$$\iint_{\mathbb{R}^{2d}} f \ln f\,\mathrm{d}x\,\mathrm{d}v\,.$$

More precisely, the associated conservation law can be written as $\partial_t \Phi(f) = \{H, \Phi(f)\}$, which is the central point in the construction of renormalized solutions by R. DiPerna and P.-L. Lions [DL88a, DL88b].

The Vlasov–Poisson equation. In the case of gravitational interactions between particles of mass m

$$K(x) = -\frac{G\,m}{|x|}$$

where G is the universal gravitational constant. In the case of interactions created by charged particles of charge q,

$$K(x) = \frac{q^2}{4\pi\varepsilon_0}\,\frac{1}{|x|}$$

so the mean-field potential is given by

$$U(t,x) = \frac{q^2}{4\pi\varepsilon_0}\int_{\mathbb{R}^d} \frac{\rho_f(y)}{|x-y|}\,\mathrm{d}y\,.$$

Taking units such that $q = \varepsilon_0 = 1$, or $G = m = 1$, we see that the pair potential solves in dimension $d = 3$

$$-\Delta K = \delta_0$$

and so the mean-field potential solves the Poisson equation

$$-\Delta U = \rho_f\,,$$

and so Equation (4) is called the Vlasov–Poisson equation in this case. Another way to write the above identity is $\operatorname{div} F = \rho_f$, which is known as the Gauss law in electromagnetism.

The Vlasov–Maxwell system. There are cases where the force is not the gradient of a potential, such as the case of electromagnetic interactions. In this case the force is called the Lorentz force and is given by the formula

$$F = q\,(E + v \times B)$$

where the electric field E and the magnetic field B are solutions of the Maxwell equations

$$\begin{cases} \operatorname{div} E = \dfrac{\rho_f}{\varepsilon_0} & \text{(Gauss' Equation)} \\ \operatorname{div} B = 0 & \text{(No magnetic charges)} \\ \operatorname{curl} E = -\partial_t B & \text{(Faraday's equation)} \\ \operatorname{curl} B = \mu_0\, q\, j + \dfrac{1}{c^2}\,\partial_t E & \text{(Ampere's equation)} \end{cases}$$

where ε_0 is the permittivity of vacuum, μ_0 is the vacuum permeability and $c^2 = 1/(\mu_0\,\varepsilon_0)$ is the speed of light.

Other Vlasov models. In the same spirit, one can build other Vlasov-type models. One can find for example relativistic Vlasov Maxwell models to take into account the effect of the relativity. The Vlasov–Navier–Stokes equation models the dynamics of particles immersed in a fluid.

2.2.3 Other Kinetic models.

All kinetic models are not mean-field models. This is due to the fact that the assumption that the force is given by a an average over a continuous distribution of particles is sometimes not well satisfied. One of such cases is the case of short length interactions. In this case, one expects that the local interactions might become dominant, which leads to the apparition of collision at a macroscopic scale.

The Botlzmann Equation. The most famous example of collisional kinetic equation is the Boltzmann equation. It is an equation of the form

$$\partial_t f + v \cdot \nabla_x f = Q_B(f, f)$$

where the quadratic form Q_B is given by

$$Q_B(f, f) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} B(v - v_*, \sigma)\,(f(v')\,f(v'_*) - f(v)\,f(v_*))\,\mathrm{d}\sigma\,\mathrm{d}v_*$$

with $f(\cdot) = f(t, x, \cdot)$, and where the post-collisional velocities are defined by

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\,\sigma \qquad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2},\,\sigma$$

for some unit vector σ, so that they satisfy the conservation of momentum $v' + v'_* = v + v_*$ and kinetic energy $|v'|^2 + |v'_*|^2 = |v|^2 + |v_*|^2$. The operator Q_B is a local function of the x variable and indicates the changes in the distribution of velocities at this point due to collisions. The kernel B of the operator depends on the chosen microscopic interaction potential. We refer to [Cer88, Vil03] for more details on this equation. One sometimes also considers the linearization of the equation around a steady state, called the linearized Boltzmann Equation, having in mind the fact that it should represent the behavior of a typical particle when the system is close to equilibrium. More simplifications lead to equations sometimes denoted as linear Boltzmann equations.

The (Linearized) Landau Equation. The Boltzmann equation does not make sense in the case of the Coulomb and gravitational potentials. In this case, another equation can be used, called the Landau equation, where the quadratic form appearing in the Boltzmann equation is replaced by

$$Q_L(f,f) = \nabla_v \cdot \int_{\mathbb{R}^d} a(v-v_*)\,(f(v_*)\,\nabla f(v) - f(v)\,\nabla f(v_*))\,\mathrm{d}v_*$$

with $a(v) = \frac{C}{|v|}\left(\mathrm{Id} - \frac{v\otimes v}{|v|^2}\right)$. Again, we refer to [Cer88, Vil03] for more details on this equation.

The Linear Fokker–Planck Equation. Another simplified model for collisional models is the Fokker–Planck equation, where the quadratic collision operator is replaced by a linear differential operator

$$\partial_t f + v\cdot\nabla_x f = \Delta_v f + \nabla_v\cdot(f\,v)\,.$$

2.3 Quantum mechanics

The goal of this section is to summarize a simplified way of understanding the axioms of quantum mechanics that we will use during the course.

2.3.1 Quick history

- In the beginning of the XX$^{\text{th}}$ century, several problems in physics are solved by the hypothesis that the energy of the light can only exist in quantified quantities depending on the wave length ν in the form of

  $$E = h\,\nu\,,$$

  the constant h in the above relation being known as the Planck constant. These problems are the study of the black body[8] radiation with its ultraviolet catastrophe solved by Planck in 1900, the Photoelectric effect[9] solved by Einstein in 1905, and the problem of the hydrogen spectral series solved by the atom model of Bohr in 1912. This suggest that light is made of particles, but it was also already known that light behaves like a wave as it produces interference patterns.

- In 1923, de Broglie makes the hypothesis that the quantization is due to the fact that every particle behave like a wave, with momentum given by

  $$|p| = m\,|v| = \frac{h}{\lambda}\,. \tag{7}$$

  The next years see the rapid development of the basis of the quantum theory (Schrödinger, Heisenberg, Born, Bohr, Dirac, Pauli, Hilbert, Von Neumann ... 1925–1927).

[8] Idealized physical body that absorbs all incident electromagnetic radiation. The black body radiation is the thermal electromagnetic radiation emitted when in thermodynamic equilibrium with its environment.

[9] Emission of electrons when electromagnetic radiation hits a material.

- At the time, the classical theory of interference was already well understood in optics. Interference of waves can be understood by associating to each wave a complex amplitude A, and then looking at the intensity obtained as the square of the sum of the complex amplitudes: $I = |A_1 + A_2|^2$. Since the light (and other particles) also produce interference patterns, the analogue of the complex amplitudes, called the wave functions, usually denoted by the letter ψ are associated to particles, and the probability of finding the particle at point x is $\rho_\psi(x) = |\psi(x)|^2$. A particle is therefore described by a complex wave function $\psi \in L^2 = L^2(\mathbb{R}^d, \mathbb{C})$ such that

$$\int_{\mathbb{R}^d} |\psi|^2 = 1\,.$$

2.3.2 Free Schrödinger equation

In light of the above quick history, it is already not difficult to understand the appearance of the free Schrödinger equation, that is the case without interactions. Let us look at the special case of a plane wave, that is a wave with a prescribed wave length. By the de Broglie relation (7), this correspond to choose a prescribed momentum. These de Broglie waves can be written

$$\psi(x) = e^{2i\pi\left(\frac{x_v}{\lambda} - \nu\, t\right)} = e^{i(x\cdot p - E\, t)/\hbar}. \tag{8}$$

For a free particle, the kinetic energy is given by $E = \frac{p^2}{2\,m}$, so $i\hbar\,\partial_t\psi = E\,\psi = \frac{|p|^2}{2\,m}\,\psi$. But one observes that $\Delta\psi = |p|^2\,\psi$, so plane waves corresponding the free particles solve the free Schrödinger equation

$$i\hbar\,\partial_t\psi = -\frac{\hbar^2}{2m}\,\Delta\psi\,. \tag{9}$$

2.3.3 Position-momentum duality

The above analysis was made using plane waves, but in the general case, we can obtain any wave function $\psi \in L^2$ as a combination of such plane waves by the Fourier inversion formula, which can be written in terms of the de Broglie waves (8) with $t = 0$,

$$\psi(x) = \int_{\mathbb{R}^d} \tfrac{1}{h^d}\,\widehat{\psi}(\tfrac{p}{h})\,e^{2i\pi\,x\cdot p/h}\,\mathrm{d}p\,.$$

Interpreting the above integral as a decomposition in terms of waves with fixed momentum, we can thus define the **momentum wave function** by

$$\varphi(p) = \frac{\widehat{\psi}(p/h)}{\|\widehat{\psi}(\cdot/h)\|_{L^2}} = \frac{1}{h^{d/2}}\,\widehat{\psi}(\tfrac{p}{h})\,,$$

where we chose the normalization so that $\|\varphi\|_{L^2} = 1$, so that again $|\varphi(p)|^2$ can be interpreted as the probability distribution of the momentum. Therefore, defining h_a the L^2-isometry $\mathsf{h}_a u(x) = a^{d/2}\,u(a\,x)$, we see that **space and momentum variables are linked by the scaled Fourier transform**[10] $\mathcal{F}_h := \mathsf{h}_{1/h}\,\mathcal{F}$.

[10] Also called sometimes the semiclassical Fourier transform

2.3.4 Observables are self-adjoint operators.

From the above considerations, one can compute the expected value for the position

$$\langle x \rangle_\psi = \int_{\mathbb{R}^d} x \, |\psi(x)|^2 \, \mathrm{d}x = \langle \psi \,|\, x \, \psi \rangle \, .$$

Similarly, the expected value for the momentum is given by

$$\begin{aligned} \langle p \rangle_\psi &= \int_{\mathbb{R}^d} p \, |\varphi(p)|^2 \, \mathrm{d}p = h^{-d} \int_{\mathbb{R}^d} p \left| \widehat{\psi}(\tfrac{p}{h}) \right|^2 \mathrm{d}p = \int_{\mathbb{R}^d} h \, y \left| \widehat{\psi}(y) \right|^2 \mathrm{d}y \\ &= \int_{\mathbb{R}^d} \overline{\widehat{\psi}}(y) \left(h \, y \, \widehat{\psi}(y) \right) \mathrm{d}y = \langle \psi \,|\, -i\hbar \nabla \, \psi \rangle \, . \end{aligned}$$

More generally, the same computations show that if $a(x)$ is a function of the position and $b(p)$ a function of the momentum, then

$$\langle a(x) \rangle_\psi = \langle \psi \,|\, a(x) \, \psi \rangle \qquad \text{and} \qquad \langle b(p) \rangle_\psi = \langle \psi \,|\, b(-i\hbar\nabla) \, \psi \rangle$$

where $b(-i\hbar\nabla)$ is defined by functional calculus, or as a Fourier multiplier by the formula $b(-i\hbar\nabla)\psi = \mathcal{F}^{-1}(hy \, \widehat{\psi}(y))$.

This leads to the more general idea that observables are associated to self-adjoint operators, whose expected value is given by

$$\langle A \rangle_\psi := \langle \psi \,|\, A\psi \rangle \, .$$

The requirement that the operators be self-adjoint correspond to ask for real-valued expected values. Indeed remember that for any self-adjoint operator A, $\langle \psi \,|\, A\psi \rangle = \overline{\langle \psi \,|\, A\psi \rangle} \in \mathbb{R}$. In particular, we have the following correspondence principle.

- An observable $a(x)$, that is a function of the position, is associated to the operator of multiplication $A\psi(x) = a(x) \, \psi(x)$. We will in general abuse of notation by writing $A = a(x)$.
- An observable $b(p)$, that is a function of the momentum, is associated to the operator $B = b(\boldsymbol{p})$, defined by functional calculus, where the **momentum operator** is defined by

  $$\boldsymbol{p} = -i\hbar\nabla \, .$$

  In $\mathbb{R}^d$, the fact that it is a Fourier multiplier can be written in terms of the semiclassical Fourier transform as $\boldsymbol{p} = \mathcal{F}_h^{-1} \, p \, \mathcal{F}_h$.

Remark 2.3.1. This allows to associate to an observable of the form $a(x) + b(p)$ the operator $A = a(x) + b(\boldsymbol{p})$. However, as will be discussed further below, this does not give a good prescription for products of operators since in general, $a(x) \, b(p) = b(p) \, a(x)$ but $a(x) \, b(\boldsymbol{p}) \neq b(\boldsymbol{p}) \, a(x)$.

Observe that $\boldsymbol{p} \in \mathcal{L}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^d, \mathbb{C}^d))$ is a vector-valued potential. On the Hilbert space $L^2(\mathbb{R}^d, \mathbb{C}^d)$, the natural scalar product is $\langle u \,|\, v \rangle = \int_{\mathbb{R}^d} \overline{u} \cdot v$, and the adjoint of $\boldsymbol{p}$ is $\boldsymbol{p}^* = -i\hbar\nabla\cdot$, where $\nabla\cdot$ is the divergence operator. In particular $|\boldsymbol{p}|^2 = \boldsymbol{p}^*\boldsymbol{p} = -\hbar^2 \, \Delta$.

2.3.5 The Schrödinger equation

According to the previous section, to the classical Hamiltonian given in (6), $H(t,x,p) = \frac{|p|^2}{2\,m} + V(t,x)$, with potential V, is associated the Hamiltonian operator

$$H = \frac{|\boldsymbol{p}|^2}{2\,m} + V = -\frac{\hbar^2}{2m}\,\Delta + V$$

where V is the operator of multiplication by the function $V(t,x)$. By analogy with the free Schrödinger equation (9), one obtains the general Schrödinger equation

$$i\hbar\,\partial_t\psi = -\frac{\hbar^2}{2m}\,\Delta\psi + V\,\psi \qquad \text{(Schrödinger)}$$

which we will better understand below.

2.3.6 Density operators.

If $\psi \in L^2$ is a wave function, then we can associate to it a density operator

$$\boldsymbol{\rho} = |\psi\rangle\,\langle\psi|\,.$$

If ψ is a solution of Schrödinger equation, then its associated operator solves the **Von Neumann equation**

$$i\hbar\,\partial_t\boldsymbol{\rho} = H\,\boldsymbol{\rho} - \boldsymbol{\rho}\,H = [H,\boldsymbol{\rho}]$$

to be put in parallel with the Vlasov equation in Poisson brackets form (5). From this analogy, one infers a correspondence principle telling us that for product of operators, one should have

$$\frac{1}{i\hbar}\,[A,B] \simeq \{a,b\}$$

for two classical quantities a and b associated to the operators A and B.

In general, instead of considering only one wave function, one can consider **mixed states** of the form

$$\boldsymbol{\rho} = \sum_{j\in J}\lambda_j\,|\psi_j\rangle\,\langle\psi_j| = \frac{1}{h^d}\sum_{j\in J}\tilde{\lambda}_j\,|\psi_j\rangle\,\langle\psi_j| \qquad (10)$$

representing a statistical incoherent superposition of **pure states**, the states associated to only one wave function. In the idea that each $\tilde{\lambda}_j$ indicates the probability of the state ψ_j, we choose

$$\sum\tilde{\lambda}_j = 1 \qquad\qquad \tilde{\lambda}_j \geq 0 \qquad\qquad \sum_{j\in J}\lambda_j = h^{-d}.$$

We will see later why there is a factor h^{-d} appearing (see Equation (19)). By the spectral theorem, this is equivalent to considering operators $\boldsymbol{\rho}$ that are compact self-adjoint operators on L^2. In particular $h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = 1$ and $\boldsymbol{\rho} \geq 0$ in the sense of operators. The expected value of an observable A in the mixed state $\boldsymbol{\rho}$ is then just the average over all the pure states

$$\langle A\rangle_{\boldsymbol{\rho}} = \sum_{j\in J}\tilde{\lambda}_j\,\langle\psi_j\,|\,A\psi_j\rangle = \sum_{k\in\mathbb{N}}\sum_{j\in J}\tilde{\lambda}_j\,\langle\psi_k\,|\,\psi_j\rangle\,\langle\psi_j\,|\,A\psi_k\rangle = h^d\,\mathrm{Tr}(A\,\boldsymbol{\rho})\,.$$

3 The Weyl quantization and the Wigner transform

In the rest of the course, we will take $m = 1$ and do the identification between momentum and velocity. In this section, we will look at the properties of the Weyl quantization and the Wigner transform, which bring a bridge between phase space statistical mechanics and quantum mechanics. We will however sometimes be rather formal and consider that the density operators are nice, and we will see in the next sections how to make rigorous the operator manipulations.

3.1 Quantization

3.1.1 Ordering of operators

How to transform a classical observable into a quantum observable? There is a priori no unique way since there is no commutation between two general operators.

Example: $x\,\boldsymbol{p} \neq \boldsymbol{p}\,x$. More precisely

$$[x, \boldsymbol{p}] = i\,\hbar\,\mathrm{Id}$$

since $\boldsymbol{p}_j\,x_k(\varphi) = -i\hbar\,\partial_j(x_k\varphi) = -i\hbar\,\delta_{j,k}\,\varphi - i\hbar\,x_k\partial_j\varphi = -i\hbar\,\delta_{j,k}\,\varphi + x_k\,\boldsymbol{p}_j\varphi$.

Idea: starting with polynomials and taking limits to get nice functions. But we have several choices

- The Kohn–Nirenberg ordering

$$x^j\,p^k \mapsto x^j\,\boldsymbol{p}^k\,.$$

- The anti Kohn–Nirenberg ordering

$$x^j\,p^k \mapsto \boldsymbol{p}^k\,x^j\,.$$

- The Weyl ordering: all the ways to multiply powers of x and $\boldsymbol{p}$. Examples:

$$x\,p \mapsto \frac{1}{2}\left(x\,\boldsymbol{p} + \boldsymbol{p}\,x\right)$$
$$x\,p^2 \mapsto \frac{1}{3}\left(x\,\boldsymbol{p}^2 + \boldsymbol{p}\,x\,\boldsymbol{p} + \boldsymbol{p}^2\,x\right)\,.$$

Advantages: Weyl ordering gives self-adjoint operators, and preserves powers of affine functions such as $(\alpha\,x + \beta\,\boldsymbol{p} + \gamma)^n$ and so also exponential functions

$$e^{\alpha x + \beta p + \gamma} \mapsto e^{\alpha x + \beta \boldsymbol{p} + \gamma}.$$

3.1.2 Weyl Quantization.

To generalize to more general operators, one can use the Fourier inversion formula[11]

$$f(x,p) = \int_{\mathbb{R}^{2d}} \widehat{f}(y,\xi)\,e^{2i\pi(y\cdot x + \xi\cdot p)}\,\mathrm{d}y\,\mathrm{d}\xi\,,$$

[11] if say $f \in L^1$ and $\widehat{f} \in L^1$, but all these formula generalize by taking a suitable weak formulation.

to deduce that the Weyl ordering should yield the following operator called the **Weyl quantization**

$$\boldsymbol{\rho}_f = \int_{\mathbb{R}^{2d}} \widehat{f}(y,\xi)\, e^{2i\pi(y\cdot x+\xi\cdot \boldsymbol{p})}\,\mathrm{d}y\,\mathrm{d}\xi\,, \tag{11}$$

The exponential of $y\cdot x+\xi\cdot\boldsymbol{p}$ can be defined through functional calculus. In general if Λ is a possibly unbounded operator that generates a semigroup, we can also define $e^{t\Lambda}u_0$ as the solution of the equation

$$\partial_t u = \Lambda u\,,$$

with initial condition $u(0,x) = u_0(x)$. This gives a simple proof of the following lemma.

Lemma 3.1 (Exponential of operators)**.** *If* $a, b \in \mathbb{C}^d$ *and* $\varphi \in L^2(\mathbb{R}^d)$*, then*

$$e^{a\cdot x+b\cdot\nabla}\varphi = e^{a\cdot(x+b/2)}\,\varphi(x+b)\,.$$

Proof. The solution of $\partial_t u = (a\cdot x+b\cdot\nabla)\,u$ is $u = u(0,x+tb)\,e^{ta\cdot(x+tb/2)}$. The result follows by taking $t=1$. ☐

In particular, $e^{2i\pi(y\cdot x+\xi\cdot\boldsymbol{p})}\varphi(x) = e^{2i\pi\,y\cdot(x+h\,\xi/2)}\,\varphi(x+h\,\xi)$. Hence for any φ

$$\boldsymbol{\rho}_f\,\varphi(x) = \int_{\mathbb{R}^{3d}} \widehat{f}(y,\xi)\,e^{2i\pi\,y\cdot(x+h\,\xi/2)}\,\varphi(x+h\,\xi)\,\mathrm{d}y\,\mathrm{d}\xi$$

and so by the Fourier inversion formula for the y variable

$$\boldsymbol{\rho}_f\,\varphi(x) = \int_{\mathbb{R}^{3d}} \mathcal{F}(f(x+h\,\xi/2,\cdot))(\xi)\,\varphi(x+h\,\xi)\,\mathrm{d}\xi$$

which can be written, with the change of variable $\xi = \frac{y-x}{h}$,

$$\boldsymbol{\rho}_f\,\varphi(x) = \tfrac{1}{h^d}\int_{\mathbb{R}^{3d}} \mathcal{F}\big(f(\tfrac{x+y}{2},\cdot)\big)\big(\tfrac{y-x}{h}\big)\,\varphi(y)\,\mathrm{d}y\,.$$

Hence we deduce that the **integral kernel of the Weyl quantization** can be written

$$\boldsymbol{\rho}_f(x,y) = \int_{\mathbb{R}^d} e^{-2i\pi(y-x)\cdot\xi}\,f(\tfrac{x+y}{2},h\xi)\,\mathrm{d}\xi = \tfrac{1}{h^d}\,\mathcal{F}\big(f(\tfrac{x+y}{2},\cdot)\big)\big(\tfrac{y-x}{h}\big)\,. \tag{12}$$

In particular, we obtain as expected a self-adjoint operator if f is a real function.

Remark 3.1.1. In comparison, the Kohn–Nirenberg ordering gives rise to the following quantization

$$f(X,D)(x,y) = \int_{\mathbb{R}^d} e^{-2i\pi(y-x)\cdot\xi}\,f(x,h\xi)\,\mathrm{d}\xi$$

which is closer to pseudo-differential operators: when $h=1$,

$$f(X,D)\varphi(x) = \int_{\mathbb{R}^d} e^{2i\pi\,x\cdot\xi}\,f(x,\xi)\,\widehat{\varphi}(\xi)\,\mathrm{d}\xi$$

i.e. $\mathcal{F}(f(X,D)\varphi(x)) = f(x,\xi)\,\widehat{\varphi}(\xi)$. It has the advantage to be local in x.

When f does not depend on x, then for any quantization, we obtain simply the Fourier multiplier

$$\mathcal{F}\Big(\boldsymbol{\rho}_{f(\xi)}\varphi(x)\Big) = f(\xi)\,\widehat{\varphi}(\xi)\,,$$

which will be written $\boldsymbol{\rho}_f = f(\boldsymbol{p})$. When it does not depend on ξ, then in the sense of distributions $\boldsymbol{\rho}_f(x,y) = \frac{1}{h^d}\, f(\frac{x+y}{2})\,\mathcal{F}(1)\big(\frac{y-x}{h}\big) = f(\frac{x+y}{2})\,\delta_0(y-x)$ and so $\boldsymbol{\rho}_{f(x)} = f(x)$ is just the multiplication operator associated to f. Another special case is the case of a factorized function $f(x)\,g(\xi)$. Then the integral kernel of the Weyl quantization takes the form

$$\boldsymbol{\rho}_{f(x)\,g(\xi)}(x,y) = \frac{1}{h^d}\,f\big(\tfrac{x+y}{2}\big)\,\widehat{g}\big(\tfrac{y-x}{h}\big)\,.$$

From any of these formulas, we see in particular that $\boldsymbol{\rho}_1 = 1$ is the identity operator on L^2.

3.1.3 Operators of Translation

One can define the operators of translation in space by $\tau_{x_0}\varphi(x) = \varphi(x - x_0)$. Then it holds

$$\tau_{x_0} = e^{-x_0\cdot\nabla_x} = e^{-i\,x_0\cdot\boldsymbol{p}/\hbar}.$$

On the other side, to obtain the operator of translation in velocity, we have to come back to the distribution of velocities $\varphi(p) = \mathcal{F}_h(\psi(x))$. We can see that the wave function associated to $\varphi(p-\xi)$ is $\psi_\xi(x) = \mathcal{F}_h^{-1}(\varphi(p-\xi)) = e^{i\,\xi_0\cdot x/\hbar}\psi(x)$. Hence the translation in velocity are given by the multiplication operators

$$\tau^{\wedge}_{\xi_0} = e^{i\,\xi_0\cdot x/\hbar} = \mathcal{F}_h^{-1}\,\tau_{\xi_0}\,.$$

Notice that these operators satisfy the semigroup identities

$$\tau_{x+x'} = \tau_x\,\tau_{x'}\,, \qquad\qquad \tau^{\wedge}_{\xi+\xi'} = \tau^{\wedge}_{\xi}\,\tau^{\wedge}_{\xi'}\,.$$

These operators are special cases of the following **phase space translation operators**

$$\tau_{z_0}\varphi = e^{i\,\xi_0\cdot\left(x-\frac{x_0}{2}\right)/\hbar}\,\varphi(x-x_0) \qquad \tau_{z_0} = e^{-i(x_0\cdot\boldsymbol{p}-\xi_0\cdot x)/\hbar} = e^{-i\,z_0^\perp\cdot\mathbf{z}/\hbar}$$

since $\tau_{(x,0)} = \tau_x$ and $\tau_{(0,\xi)} = \tau^{\wedge}_{\xi}$. Here, $\mathbf{z} = (x,\boldsymbol{p})$ and $z_0^\perp = (-\xi_0, z_0)$ so $z_0^\perp\cdot\mathbf{z} = x_0\cdot\xi - x\cdot\xi_0$ is the symplectic product. One sometimes also defines the **Weyl operators**

$$W_{z_0} = e^{2i\pi(\xi_0\cdot x + x_0\cdot\boldsymbol{p})} = e^{2i\pi\,z_0\cdot\mathbf{z}} = \tau_{hz_0^\perp}\,.$$

All these operators are unitary so $\tau_z^{-1} = \tau_{-z} = \tau_z^*$. Notice that $\tau_x\,\tau^{\wedge}_{\xi} = e^{-i\,x\cdot\xi/\hbar}\,\tau^{\wedge}_{\xi}\tau_x$ and $\tau_z \neq \tau_x\,\tau^{\wedge}_{\xi}$. More precisely, it holds

$$\tau_z = \tau^{\wedge}_{\frac{\xi}{2}}\,\tau_x\,\tau^{\wedge}_{\frac{\xi}{2}} = \tau_{\frac{x}{2}}\,\tau^{\wedge}_{\xi}\,\tau_{\frac{x}{2}}\,.$$

From this relation and the commutation relation between τ and $\tau^{\wedge}$ we get

$$\tau_{z+z'} = e^{-i\pi\left(x\cdot\xi'-x'\cdot\xi\right)/h}\,\tau_z\tau_{z'} = e^{-i\,\pi\,z^\perp\cdot z'/h}\,\tau_z\tau_{z'}. \tag{13}$$

To work with density operators instead of wave functions, it makes sense to define the operators $\mathsf{T}_{z_0} \in \mathcal{L}(\mathcal{L}(\mathcal{H}))$ acting on observables and density operators by doing the conjugation by the translation operators

$$\mathsf{T}_{z_0}\boldsymbol{\rho} := \tau_{z_0}\,\boldsymbol{\rho}\,\tau_{-z_0}\,. \tag{14}$$

They satisfy $\mathsf{T}_{z_0+z_1} = \mathsf{T}_{z_0}\,\mathsf{T}_{z_1} = \mathsf{T}_{z_1}\,\mathsf{T}_{z_0}$. For the position and momentum operators, it gives naturally

$$\mathsf{T}_{z_0} x = x - x_0 \qquad\qquad \mathsf{T}_{z_0}\boldsymbol{p} = \boldsymbol{p} - \xi_0$$

which can be written $\mathsf{T}_{z_0}\mathbf{z} = \mathbf{z} - z_0$. More generally, they translate any Weyl quantization, i.e.

$$\mathsf{T}_{z_0}\,\boldsymbol{\rho}_f = \boldsymbol{\rho}_{f(\cdot - z_0)}. \tag{15}$$

Proof. Using the inverse Fourier transform type definition of the Weyl quantization (11), yields

$$\boldsymbol{\rho}_f = \int_{\mathbb{R}^d} \widehat{f}(z)\,\tau_{hz^\perp}\,\mathrm{d}z. \tag{16}$$

Now using two times Formula (13),

$$\tau_{z_0}\,\tau_{hz^\perp}\,\tau_{-z_0} = e^{i\pi\left(h\,z_0^\perp\cdot z^\perp - (z_0 + hz^\perp)^\perp\cdot z_0\right)/h}\,\tau_{hz^\perp} = e^{2i\pi\,z_0\cdot z}\,\tau_{hz^\perp}$$

and so by the usual property of the Fourier transform,

$$\tau_{z_0}\,\boldsymbol{\rho}\,\tau_{-z_0} = \int_{\mathbb{R}^d} \widehat{f}(z)\,e^{2i\pi\,z_0\cdot z}\,\tau_{hz^\perp}\,\mathrm{d}z = \int_{\mathbb{R}^d} \widehat{f}(z - z_0)\,\tau_{hz^\perp}\,\mathrm{d}z$$

which leads to the result thanks to Equation (15). □

3.2 Wigner transform

3.2.1 Definition

Now we want conversely to associate to an operator a function of the phase space. We just have to solve the above equation (12) for f. Doing the change of variable

$$\begin{cases} y' = \dfrac{x-y}{h} \\ x' = \dfrac{x+y}{2} \end{cases} \qquad \Longleftrightarrow \qquad \begin{cases} x = x' + \dfrac{h\,y'}{2} \\ y = x' - \dfrac{h\,y'}{2} \end{cases}$$

we deduce

$$\begin{aligned} \boldsymbol{\rho} = \boldsymbol{\rho}_f \;&\Longleftrightarrow\; \boldsymbol{\rho}_f\!\left(x + \frac{h\,y}{2}, x - \frac{h\,y}{2}\right) = \tfrac{1}{h^d}\,\mathcal{F}(f(x,\cdot))(-y) \\ &\Longleftrightarrow\; \boldsymbol{\rho}_f\!\left(x + \frac{h\,y}{2}, x - \frac{h\,y}{2}\right) = \tfrac{1}{h^d}\,\mathcal{F}^{-1}(f(x,\cdot))(y) \\ &\Longleftrightarrow\; f(x,\xi) = h^d \int_{\mathbb{R}^d} e^{-2i\pi\,y\cdot\xi}\,\boldsymbol{\rho}_f\!\left(x + \frac{h\,y}{2}, x - \frac{h\,y}{2}\right)\mathrm{d}y \end{aligned}$$

and so we define the **Wigner transform** by

$$f_{\boldsymbol{\rho}}(x,\xi) = \int_{\mathbb{R}^d} e^{-i\,y\cdot\xi/\hbar}\,\boldsymbol{\rho}(x + \tfrac{y}{2}, x - \tfrac{y}{2})\,\mathrm{d}y = \mathcal{F}\big(\boldsymbol{\rho}(x + \tfrac{\cdot}{2}, x - \tfrac{\cdot}{2})\big)\Big(\tfrac{\xi}{h}\Big). \tag{17}$$

Notice that the expression using the Fourier transform can be defined more generally for tempered distributions.

Remark 3.2.1. For a pure state $\boldsymbol{\rho} = h^{-d}\,|\psi\rangle\,\langle\psi|$, we define

$$f_\psi(x,\xi) = \frac{1}{h^d}\int_{\mathbb{R}^d} e^{-i\,y\cdot\xi/\hbar}\,\psi(x + \tfrac{y}{2})\,\overline{\psi}(x - \tfrac{y}{2})\,\mathrm{d}y = \mathcal{F}_y\Big(\psi(x + \tfrac{hy}{2})\,\overline{\psi}(x - \tfrac{hy}{2})\Big)(\xi)\,.$$

3.2.2 Basic properties

As expected, the Wigner transform of a self-adjoint operator is real. More precisely

$$f_{\boldsymbol{\rho}^*} = \overline{f_{\boldsymbol{\rho}}}\,.$$

One can also notice that $f_{\boldsymbol{\rho}^\top}(x,\xi) = f_{\boldsymbol{\rho}}(x,-\xi)$. The Wigner transform commutes well with translation operators, since it follows from Identity (15) that

$$f_{\mathsf{T}_{z_0}\boldsymbol{\rho}}(x,\xi) = f_{\boldsymbol{\rho}}(z-z_0)\,, \tag{18}$$

In particular, $f_{\boldsymbol{\rho}}(z) = f_{\tau_{-z}\boldsymbol{\rho}\tau_z}(0)$, so the Wigner transform is in some sense a translation in phase space of the kernel of the operator.

Spatial observables. To compute the phase space integral of the Wigner transform, it suffices to use the definition (17) of the Wigner transform in terms of the Fourier transform, and the fact that the integral of the Fourier transform is its value at 0. It yields

$$\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi = h^d \int_{\mathbb{R}^d} \boldsymbol{\rho}(x,x)\,\mathrm{d}x\,.$$

Therefore, if $\boldsymbol{\rho} = \sum_{j\in J} \lambda_j \left|\psi_j\right\rangle \left\langle\psi_j\right|$ is a nice compact self-adjoint operator,

$$\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi = h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = \sum_{j\in J}\lambda_j \tag{19}$$

and so we understand the h^{-d} that was appearing in Formula (10). The generalization of the **position density** $\rho_\psi(x) = \left|\psi(x)\right|^2$ for pure states is now given by

$$\rho_{\boldsymbol{\rho}}(x) = \int_{\mathbb{R}^d} f_{\boldsymbol{\rho}}\,\mathrm{d}\xi = \sum_{j\in J}\lambda_j \left|\psi_j(x)\right|^2 = h^d\,\boldsymbol{\rho}(x,x)$$

and more generally, this operation can be seen as the analogue of the integral with respect to the momentum variable. In particular, for any observable depending only on the position $A(x)$, identified with the operator of multiplication by A,

$$\left\langle A(x)\right\rangle_{\boldsymbol{\rho}} = h^d\,\mathrm{Tr}(A(x)\boldsymbol{\rho}) = \int_{\mathbb{R}^d} A(x)\,\rho_{\boldsymbol{\rho}}(x)\,\mathrm{d}x = \iint_{\mathbb{R}^{2d}} A(x)\,f_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi\,.$$

Fourier transform and momentum observables. From the Fourier inversion formula, we immediately get

$$\mathcal{F}_\xi(f_{\boldsymbol{\rho}})(x,\xi) = h^d\,\boldsymbol{\rho}(x-\tfrac{h\xi}{2}, x+\tfrac{h\xi}{2})\,.$$

On the other hand

$$\begin{aligned}\mathcal{F}_x(f_{\boldsymbol{\rho}}) &= \iint_{\mathbb{R}^{2d}} e^{-2i\pi(y\cdot\xi/h+\eta\cdot x)}\,\boldsymbol{\rho}(\eta+\tfrac{y}{2},\eta-\tfrac{y}{2})\,\mathrm{d}y\,\mathrm{d}\eta\\ &= \iint_{\mathbb{R}^{2d}} e^{-2i\pi((\eta-y)\cdot\xi/h+x\cdot(\eta+y)/2)}\,\boldsymbol{\rho}(\eta,y)\,\mathrm{d}y\,\mathrm{d}\eta\\ &= \overset{\curlywedge}{\boldsymbol{\rho}}(\tfrac{\xi}{h}+\tfrac{x}{2},\tfrac{\xi}{h}-\tfrac{x}{2})\end{aligned}$$

where

$$\overset{\curlywedge}{\boldsymbol{\rho}} = \mathcal{F}\,\boldsymbol{\rho}\,\mathcal{F}^{-1} = \sum_{j\in J} \lambda_j\,|\widehat{\psi_j}\rangle\,\langle\widehat{\psi_j}| \geq 0$$

is the operator with kernel $\overset{\curlywedge}{\boldsymbol{\rho}}(x,y) = \mathcal{F}_x\,\mathcal{F}_y^{-1}\,\boldsymbol{\rho}(x,y)$. Once again, this is the application of the fact that $\mathcal{F}_h$ exchanges position and momentum. In particular, evaluating $\mathcal{F}_x(f_{\boldsymbol{\rho}})$ at $x=0$, we see that the generalization of the momentum density $h^{-d}\,|\widehat{\psi}(\frac{\xi}{h})|^2$ is

$$\int_{\mathbb{R}^d} f_{\boldsymbol{\rho}}\,\mathrm{d}x = \overset{\curlywedge}{\boldsymbol{\rho}}(\tfrac{\xi}{h},\tfrac{\xi}{h}) = \sum_{j\in J}\lambda_j\left|\widehat{\psi_j}(\tfrac{\xi}{h})\right|^2.$$

From the above formula is deduced without difficulty that observables $B(\boldsymbol{p})$ depending only on the momentum can then be evaluated by writing

$$\langle B(\boldsymbol{p})\rangle_{\boldsymbol{\rho}} = h^d\,\mathrm{Tr}(B(\boldsymbol{p})\,\boldsymbol{\rho}) = \iint_{\mathbb{R}^{2d}} B(\xi)\,f_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi$$

and in particular the kinetic energy reads

$$\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,|\xi|^2\,\mathrm{d}x\,\mathrm{d}\xi = h^d\,\mathrm{Tr}\Big(|\boldsymbol{p}|^2\,\boldsymbol{\rho}\Big) = h^d\sum_{j\in J}\lambda_j\int_{\mathbb{R}^d}|\nabla\psi_j|^2.$$

L^2 **norm.** By the isometric property of the Fourier transform

$$\int_{\mathbb{R}^d}|f_{\boldsymbol{\rho}}(x,\xi)|^2\,\mathrm{d}\xi = h^d\,\big\|\boldsymbol{\rho}(x+\tfrac{y}{2},x-\tfrac{y}{2})\big\|^2_{L^2_y}.$$

Therefore, noticing that the change of variable $(x+y/2,x-y/2)\mapsto(x,y)$ has Jacobian 1, we get

$$\|f_{\boldsymbol{\rho}}\|_{L^2(\mathbb{R}^d)} = h^{d/2}\,\|\boldsymbol{\rho}\|_2 = \Big(h^d\,\mathrm{Tr}\Big(|\boldsymbol{\rho}|^2\Big)\Big)^{1/2}.$$

More generally, the scalar product becomes

$$\big\langle f_{\boldsymbol{\rho}}\,\big|\,f_{\boldsymbol{\rho}_2}\big\rangle = h^d\,\mathrm{Tr}(\boldsymbol{\rho}^*\boldsymbol{\rho}_2)\,. \tag{20}$$

Proof. Using the fact that the Fourier transform preserves the hermitian scalar product and doing the same change of variable of Jacobian 1 as above, we obtain

$$\begin{aligned}\int_{\mathbb{R}^{2d}}\overline{f_{\boldsymbol{\rho}_1}}\,f_{\boldsymbol{\rho}_2} &= \int_{\mathbb{R}^{2d}}\overline{\mathcal{F}\big(\boldsymbol{\rho}_1(x+\tfrac{\cdot}{2},x-\tfrac{\cdot}{2})\big)\Big(\tfrac{\xi}{h}\Big)}\,\mathcal{F}\big(\boldsymbol{\rho}_2(x+\tfrac{\cdot}{2},x-\tfrac{\cdot}{2})\big)\Big(\tfrac{\xi}{h}\Big)\,\mathrm{d}z\\ &= h^d\int_{\mathbb{R}^{2d}}\overline{\boldsymbol{\rho}_1(x,y)}\,\boldsymbol{\rho}_2(x,y)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

and we conclude using the formula of the trace for nice integral operators. □

From Formula (20), we also get

$$\langle f_{\boldsymbol{\rho}}\,|\,g\rangle = h^d\,\mathrm{Tr}\big(\boldsymbol{\rho}^*\,\boldsymbol{\rho}_g\big) \tag{21}$$

which shows another link between the Wigner transform and the Weyl quantization. From the representation (11) of the Weyl quantization, it allows to get another formula for the Wigner transform

$$\langle f_{\boldsymbol{\rho}}\,|\,\varphi\rangle = h^d\int_{\mathbb{R}^d}\mathrm{Tr}\big(\boldsymbol{\rho}^*\,e^{2i\pi\,z\cdot\mathbf{z}}\big)\,\widehat{\varphi}(z)\,\mathrm{d}z$$

which can also be written

$$\widehat{f_{\boldsymbol{\rho}}}(z) = h^d \operatorname{Tr}\!\left(e^{-2i\pi\, z\cdot\mathbf{z}}\, \boldsymbol{\rho}\right). \tag{22}$$

This is the analogue of the integral formula for the Fourier transform but expressed in terms of the trace, called the Groenewold formula [Gro46].

Positivity. The Wigner transform of a self-adjoint operator is real. However, the Wigner transform of a positive operator is not necessarily non-negative. It is however possible to rewrite the condition $\boldsymbol{\rho} \geq 0$. For any $\varphi \in L^2$,

$$\langle \varphi \,|\, \boldsymbol{\rho}\, \varphi \rangle = \iint_{\mathbb{R}^{2d}} \boldsymbol{\rho}(x,y)\, \overline{\varphi(x)}\, \varphi(y) \,\mathrm{d}x \,\mathrm{d}y = \int_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\, f_\varphi$$

so

$$\boldsymbol{\rho} \geq 0 \qquad \Longleftrightarrow \qquad \forall \varphi \in L^2, \int_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\, f_\varphi \geq 0\,. \tag{23}$$

Husimi transform. Let $z = (x,\xi)$, $z_0 = (x_0, \xi_0) \in \mathbb{R}^{2d}$ and define the Gaussian coherent state centered around z_0 by

$$\psi_{z_0}(x) = \left(\tfrac{2}{h}\right)^{d/4} e^{-|x-x_0|^2/(2\hbar)}\, e^{i\,\xi_0\cdot\left(x-\frac{x_0}{2}\right)/\hbar} = \tau_{z_0}\psi_0(x)$$

and its corresponding density operator by $\boldsymbol{\rho}_{z_0} = h^{-d}\, |\psi_{z_0}\rangle\, \langle\psi_{z_0}|$. Then

$$f_{\boldsymbol{\rho}_{z_0}}(z) = g_h(z-z_0) \qquad\qquad \text{with} \qquad\qquad g_h(z) = (2/h)^d\, e^{-|z|^2/\hbar}. \tag{24}$$

Notice that g_h is a Gaussian approximation of the Dirac delta.

Proof. By Equation (18), it is sufficient to look at the case $z_0 = 0$. Then

$$\begin{aligned}
f_{\boldsymbol{\rho}_0}(z) &= \frac{2^{d/2}}{h^{3d/2}} \int_{\mathbb{R}^d} e^{-i\,y\cdot\xi/\hbar}\, e^{-\left(|x+y/2|^2+|x-y/2|^2\right)/(2\hbar)} \,\mathrm{d}y \\
&= \frac{2^{d/2}}{h^{3d/2}}\, e^{-|x|^2/\hbar} \int_{\mathbb{R}^d} e^{-i\,y\cdot\xi/\hbar}\, e^{-|y|^2/(4\hbar)} \,\mathrm{d}y \\
&= \frac{2^{d/2}}{h^{3d/2}}\, e^{-|x|^2/\hbar}\, \mathcal{F}\!\left(e^{-\pi|y|^2/(2\,h)}\right)\left(\tfrac{\xi}{h}\right)
\end{aligned}$$

and the result follows by the formula of the Fourier transform for a Gaussian. □

Hence, defining the **Husimi transform** as the convolution of the Wigner function with a Gaussian, it gives a nonnegative function (see e.g. [LP93, Equation (25)])

$$\tilde{f}_{\boldsymbol{\rho}} = g_h * f_{\boldsymbol{\rho}} \geq 0\,.$$

Proof. By Criterion (23) and Formula (24), $\tilde{f}_{\boldsymbol{\rho}}(z_0) = \int_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\, f_{\boldsymbol{\rho}_{z_0}} \geq 0$. □

Remark 3.2.2. One can actually prove that the only positive Wigner transforms of pure states are Gaussians (see [Hud74]).

Remark 3.2.3. The positivity of the Husimi allows to have a simple criterion for the finiteness of the trace of $\boldsymbol{\rho}$ since

$$\big\|\tilde{f}_{\boldsymbol{\rho}}\big\|_{L^1} = \int_{\mathbb{R}^{2d}} g_h * f_{\boldsymbol{\rho}} = \int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}} = h^d \operatorname{Tr}(\boldsymbol{\rho})\,.$$

Dynamics. It is a remarkable fact that if $\boldsymbol{\rho}$ solves the free Schrödinger equation (the free Von Neumann equation)

$$i\hbar\,\partial_t\boldsymbol{\rho} = \left[\tfrac{|\boldsymbol{p}|^2}{2}, \boldsymbol{\rho}\right]$$

then $f_{\boldsymbol{\rho}}$ solves the free transport equation

$$\partial_t f_{\boldsymbol{\rho}} + \xi\cdot\nabla_x f_{\boldsymbol{\rho}} = 0\,.$$

Proof. This follows from the fact that

$$\begin{aligned}\xi\cdot\nabla_x f_{\boldsymbol{\rho}} &= i\hbar\int_{\mathbb{R}^d}\nabla_y\left(e^{-i\,y\cdot\xi/\hbar}\right)\cdot(\nabla_1+\nabla_2)\,\boldsymbol{\rho}(x+\tfrac{y}{2}, x-\tfrac{y}{2})\,\mathrm{d}y\\ &= -i\,\frac{\hbar}{2}\int_{\mathbb{R}^d} e^{-i\,y\cdot\xi/\hbar}\,(\nabla_1-\nabla_2)\cdot(\nabla_1+\nabla_2)\,\boldsymbol{\rho}(x+\tfrac{y}{2}, x-\tfrac{y}{2})\,\mathrm{d}y\end{aligned}$$

where ∇_1 denotes the gradient with respect to the first variable of $\boldsymbol{\rho}$, and noticing that $(\nabla_1-\nabla_2)\cdot(\nabla_1+\nabla_2)\,\boldsymbol{\rho}(x,y) = (\Delta_1-\Delta_2)\,\boldsymbol{\rho}(x,y) = [\Delta,\boldsymbol{\rho}]\,(x,y)$ is the integral kernel of the operator $[\Delta,\boldsymbol{\rho}]$. ☐

On the other hand, if the Hamiltonian contains a potential $H = \frac{|\boldsymbol{p}|^2}{2} + V$, then the Wigner transform of $\boldsymbol{\rho}$ satisfies

$$\partial_t f_{\boldsymbol{\rho}} + \xi\cdot\nabla_x f_{\boldsymbol{\rho}} + \mathcal{K}_h \underset{\xi}{*} f_{\boldsymbol{\rho}} = 0\,,$$

where

$$\mathcal{K}_h = 2i\pi\int_{\mathbb{R}^d} e^{-2i\pi y\cdot\xi}\,\frac{V(x+hy/2)-V(x-hy/2)}{h}\,\mathrm{d}y\,.$$

Proof. Since

$$\frac{1}{i\hbar}\,f_{[V,\boldsymbol{\rho}]} = \mathcal{F}\bigg(\frac{V(x+hy/2)-V(x-hy/2)}{i\hbar}\,\boldsymbol{\rho}(x+\tfrac{hy}{2}, x-\tfrac{hy}{2})\bigg)\,(\xi)$$

the result follows for the fact that the Fourier transform of a product is the convolution of the Fourier transforms. ☐

In particular, at least formally, when $h\to 0$, $\mathcal{K}_h$ converges to

$$\mathcal{K}_0 = -\nabla V\cdot\nabla\delta_0(\xi)$$

and so one might expect $f_{\boldsymbol{\rho}}$ to converge to a solution of the Vlasov equation. But the first difficulty is that $f_{\boldsymbol{\rho}}$ is not positive in general and so $\int_{\mathbb{R}^{2d}}|f_{\boldsymbol{\rho}}|$ and $\|f_{\boldsymbol{\rho}}\|_{L^\infty}$ are not conserved quantities. One however still have conservation of the total mass $h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = \iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}$ and the $L^2(\mathbb{R}^{2d})$ norm since

$$i\hbar\,\partial_t\boldsymbol{\rho}^2 = \left[H_{\boldsymbol{\rho}}, \boldsymbol{\rho}^2\right]$$

and for nice operators, the trace of a commutator is 0. Similarly, if V is time independent, then the energy

$$h^d\,\mathrm{Tr}(H\boldsymbol{\rho}) = \frac{1}{2}\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,|\xi|^2\,\mathrm{d}x\,\mathrm{d}\xi + \int_{\mathbb{R}^d}\rho_{\boldsymbol{\rho}}\,V$$

is conserved since $h^d\,\mathrm{Tr}(H\,[H,\boldsymbol{\rho}]) = h^d\,\mathrm{Tr}\big(H^2\boldsymbol{\rho} - H\boldsymbol{\rho}H\big) = 0$. When V is a mean-field potential, that is $V = V_{\boldsymbol{\rho}} = K * \rho_{\boldsymbol{\rho}}$, then it is time dependent but by symmetry in the integral defining the potential energy

$$\int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}\,\partial_t V_{\boldsymbol{\rho}} = \frac{1}{2}\int_{\mathbb{R}^d} (K * \partial_t\rho_{\boldsymbol{\rho}})\,\rho_{\boldsymbol{\rho}} + (K * \rho_{\boldsymbol{\rho}})\,\partial_t\rho_{\boldsymbol{\rho}} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}\,V_{\boldsymbol{\rho}}$$

and so the conserved energy is

$$\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,|\xi|^2\,\mathrm{d}x\,\mathrm{d}\xi + \int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}\,V_{\boldsymbol{\rho}}\,.$$

3.2.3 Wigner Measures

We suppose $(\boldsymbol{\rho})_{h>0} = (\boldsymbol{\rho}_h)_{h>0}$ is a sequence of operators such that $h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = \int_{\mathbb{R}^d}\rho_{\boldsymbol{\rho}}$ is bounded uniformly in $\hbar$. Then what can happen when $h \to 0$? From Remark 3.2.3, we see that $\big\|\tilde{f}_{\boldsymbol{\rho}}\big\|_{L^1}$ is bounded uniformly in $\hbar$ and so there exists a sequence $h_n \to 0$ and a measure $\mu \in \mathcal{M}(\mathbb{R}^{2d})$ that we call a **Wigner measure** such that

$$\tilde{f}_{\boldsymbol{\rho}} \underset{h_n\to 0}{\rightharpoonup} \mu \geq 0 \tag{25}$$

weakly in the sense of measures. To obtain uniform bounds on the Wigner measure, following Lions–Paul [LP93], one can introduce the separable Banach algebra of test functions

$$\mathcal{A} = \{\,\varphi \in C_0^0(\mathbb{R}^{2d}), \|\varphi\|_{\mathcal{A}} := \|\mathcal{F}_\xi\,\varphi\|_{L^1_\xi L^\infty_x} < \infty\,\}\,.$$

Theorem 3.2 (Lions–Paul [LP93])**.** *Let $M_0 > 0$ and $(\boldsymbol{\rho})_{h>0} = (\boldsymbol{\rho}_h)_{h>0}$ be a family of positive operators such that $h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = M_0$. Then for every $h > 0$,*

$$\|f_{\boldsymbol{\rho}}\|_{\mathcal{A}'} \leq M_0 \tag{26}$$

and there exists a sequence $h = (h_n)_{n\in\mathbb{N}} \to 0$ such that

$$f_{\boldsymbol{\rho}} \underset{h\to 0}{\rightharpoonup} \mu \geq 0$$

in the weak-$*$ topology of $\mathcal{A}'$. It satisfies

$$\iint_{\mathbb{R}^{2d}} \mu \leq \liminf_{h\to 0} \int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}(x)\,\mathrm{d}x\,. \tag{27}$$

Remark 3.2.4. In particular, even if Wigner transforms are not always positive, it is the case in the limit. Notice also that since $H^s(\mathbb{R}^{2d}) \subset \mathcal{A} \subset C_0^0(\mathbb{R}^{2d})$ for any $s > d$, we have the following inclusions $\mathcal{M}(\mathbb{R}^{2d}) \subset \mathcal{A}' \subset H^{-s}(\mathbb{R}^{2d})$. In particular $\mathcal{A}'$ contains distributions that are not measures, but some sequences of Wigner transforms will still always converge to measures.

Proof. We denote by $\varphi = \varphi(x,\xi)$ the test function in $\mathcal{A}$ and by $\widehat{\varphi} := \mathcal{F}_\xi\,\varphi$. We first notice that

$$\begin{aligned}\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\,\varphi\,\mathrm{d}x\,\mathrm{d}\xi &= \iint_{\mathbb{R}^{2d}} \boldsymbol{\rho}(x+\tfrac{y}{2}, x-\tfrac{y}{2})\,\widehat{\varphi}(x,y/h)\,\mathrm{d}x\,\mathrm{d}y \\ &\leq \sup_y \left(\int_{\mathbb{R}^d} \sum_{j\in J} \lambda_j\,\psi_j(x+\tfrac{y}{2})\,\overline{\psi_j(x-\tfrac{y}{2})}\,\mathrm{d}x\right)\int_{\mathbb{R}^d}\sup_x|\widehat{\varphi}(x,y/h)|\,\mathrm{d}y\,.\end{aligned}$$

Thus Inequality (26) follows by the Cauchy–Schwarz inequality. From this uniform bound, we deduce that $f_{\boldsymbol{\rho}}$ converges up to a subsequence to a measure $\mu \in \mathcal{M}(\mathbb{R}^{2d})$. Up to taking a subsequence of this subsequence, we can assume that the convergence of the Husimi measure (25) holds as well. Now observe that by definition of the Husimi transform and by Inequality (26)

$$\left\langle f_{\boldsymbol{\rho}} - \tilde{f}_{\boldsymbol{\rho}}, \varphi \right\rangle_{\mathcal{A}',\mathcal{A}} = \left\langle f_{\boldsymbol{\rho}}, \varphi - g_h * \varphi \right\rangle_{\mathcal{A}',\mathcal{A}} \leq M_0 \left\| \varphi - g_h * \varphi \right\|_{\mathcal{A}}$$

and since $\mathcal{F}_\xi(g_h * \varphi) = (g_h(x) * \widehat{\varphi})\, e^{-\pi h|\xi|^2/2}$, it holds

$$\left\| \varphi - g_h * \varphi \right\|_{\mathcal{A}} \leq I_1 + I_2$$

where

$$I_1 = \int_{\mathbb{R}^d} \left(1 - e^{-\frac{\pi}{2}h|\xi|^2}\right) \sup_x |\widehat{\varphi}| \,\mathrm{d}\xi$$

$$I_2 = \int_{\mathbb{R}^d} \sup_x |\widehat{\varphi} - g_h(x) * \widehat{\varphi}| \,\mathrm{d}\xi = \int_{\mathbb{R}^d} \sup_x \left| \int_{\mathbb{R}^d} \left(\widehat{\varphi}(x,\xi) - \widehat{\varphi}(x-y,\xi)\right) g_h(y) \,\mathrm{d}y \right| \mathrm{d}\xi$$

both converge to 0 by dominated convergence, and the fact that for any function $u \in C^0_0$, $g_h * u \to u$ almost everywhere. Inequality (27) follows from the weak convergence of the Husimi transform to μ. ☐

Similarly, $\rho_{\boldsymbol{\rho}}(x) = h^d\, \boldsymbol{\rho}(x,x) \geq 0$ satisfies $\|\rho_{\boldsymbol{\rho}}\|_{L^1} = 1$ and so converges weakly to a measure ρ up to a subsequence. Recall that a sequence of nonnegative bounded measures $\mu_n \in \mathcal{M}(\mathbb{R}^d)$ is said to be tight if and only if

$$\sup_{n\in\mathbb{N}} \mu_n(\{\, |x| > R \,\}) = \sup_{n\in\mathbb{N}} \int_{|x|>R} \mu_n \underset{R\to\infty}{\longrightarrow} 0\,.$$

Proposition 3.3. *If $\rho_{\boldsymbol{\rho}} \rightharpoonup \rho$ and $\tilde{f}_{\boldsymbol{\rho}} \rightharpoonup \mu$ when $h \to 0$ (or a subsequence), then in the sense of measures*

$$\rho \geq \rho_\mu := \int_{\mathbb{R}^d} \mu(\cdot, \mathrm{d}\xi)\,, \tag{28}$$

with equality if and only if the sequence of function (depending on h)

$$\int_{\mathbb{R}^d} f_{\boldsymbol{\rho}} \,\mathrm{d}x = \check{\boldsymbol{\rho}}(\tfrac{\xi}{h}, \tfrac{\xi}{h}) = \sum_{j\in J} \lambda_j \left|\widehat{\psi_j}(\tfrac{\xi}{h})\right|^2$$

is tight. In particular, equality holds in Inequality (28) if for some $\alpha > 0$, the value of

$$\iint_{\mathbb{R}^{2d}} f_{\boldsymbol{\rho}}\, |\xi|^\alpha \,\mathrm{d}x\,\mathrm{d}\xi = h^d\, \mathrm{Tr}(|\boldsymbol{p}|^\alpha\, \boldsymbol{\rho}) = h^d \sum_{j\in J} \lambda_j \int_{\mathbb{R}^d} \left|(\hbar\Delta)^{\frac{\alpha}{2}} \psi_j\right|^2$$

is bounded uniformly with respect to $\hbar$.

Proof. If $\rho_{\boldsymbol{\rho}}$ converges weakly to ρ, then $\tilde{\rho}_{\boldsymbol{\rho}}(x) := \int_{\mathbb{R}^d} \tilde{f}_{\boldsymbol{\rho}_{\boldsymbol{\rho}}} \,\mathrm{d}\xi = \rho_{\boldsymbol{\rho}} * g_h(x) \rightharpoonup \rho(x)$. Defining $\chi_R \in C^\infty_c$ such that $0 \leq \chi_R \leq 1$ and $\chi_R = 1$ on $B(0,R)$, since $\tilde{f}_{\boldsymbol{\rho}} \geq 0$, it holds

$$\int_{\mathbb{R}^d} \varphi(x)\, \tilde{\rho}_{\boldsymbol{\rho}}(x) \,\mathrm{d}x \geq \iint_{\mathbb{R}^{2d}} \chi_R(\xi)\, \varphi(x)\, \tilde{f}_{\boldsymbol{\rho}}(x,\xi) \,\mathrm{d}x\,\mathrm{d}\xi\,.$$

Here we can pass to the limit $h \to 0$ and by weak convergence

$$\int_{\mathbb{R}^d} \varphi(x)\,\rho(x)\,\mathrm{d}x \geq \iint_{\mathbb{R}^{2d}} \chi_R(\xi)\,\varphi(x)\,\mu(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi$$

and so by letting $R \to 0$, we deduce that $\rho \geq \rho_\mu$ in the sense of distributions. If $\int_{\mathbb{R}^d} f_{\boldsymbol{\rho}}\,\mathrm{d}x$ is tight, then $\int_{\mathbb{R}^d} \tilde{f}_{\boldsymbol{\rho}}\,\mathrm{d}x$ is tight and so

$$\sup_{h\geq 0} \iint_{\mathbb{R}^{2d}} (1-\chi_R(\xi))\,\tilde{f}_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi \underset{R\to\infty}{\longrightarrow} 0$$

which implies that $\rho_{\boldsymbol{\rho}} \to \rho_\mu$ in the sense of distributions. □

From another point of view, we also see that since $\boldsymbol{\rho} = \boldsymbol{\rho}_h$ is a positive Hilbert–Schmidt operator, $\left\|h^d\boldsymbol{\rho}\right\|_{L^2(\mathbb{R}^{2d})} = \left\|h^d\boldsymbol{\rho}\right\|_2 \leq h^d\,\mathrm{Tr}(\boldsymbol{\rho}) = M_0$. Hence $\boldsymbol{\mu}_h := h^d\boldsymbol{\rho}$ also converges weakly (up to subsequence) to an Hilbert–Schmidt operator $\boldsymbol{\mu}_\circ$ in $L^2(\mathbb{R}^{2d})$.

Proposition 3.4. *Let $\boldsymbol{\mu}_h = h^d\,\boldsymbol{\rho} = |\psi\rangle\,\langle\psi|$ for a fixed function $\psi \in L^2(\mathbb{R}^d)$ independent of h. Then the Wigner measure associated to $\boldsymbol{\rho}$ satisfies*

$$\mu(x,\xi) \geq \rho_\circ(x)\,\delta_0(\xi)$$

where $\rho_\circ(x) = \boldsymbol{\mu}_\circ(x,x)$. In particular $\rho_\mu(x) \geq \rho_\circ(x)$ and so

$$\int_{\mathbb{R}^{2d}} \mu(z)\,\mathrm{d}z \geq \mathrm{Tr}(\boldsymbol{\mu})\,.$$

Remark 3.2.5. Notice that here $\mathrm{Tr}(\boldsymbol{\mu}_h) = 1$. Of course if $\|f_{\boldsymbol{\rho}}\|_{L^2} = h^{d/2}\,\|\boldsymbol{\rho}\|_2 \leq C$ uniformly in $\hbar$, then $\|\boldsymbol{\mu}_h\|_2 = h^d\,\|\boldsymbol{\rho}\|_2 \leq C\,h^{d/2}$ and $\boldsymbol{\mu}_\circ = 0$, in which case the above proposition does not bring any interesting information.

Proof. Notice that

$$\boldsymbol{\mu}_\circ\Big(x + \tfrac{hy}{2}, x - \tfrac{hy}{2}\Big) \underset{h\to 0}{\rightharpoonup} \boldsymbol{\mu}_\circ(x,x) = \rho_\circ(x)$$

in the sense of tempered distribution in $\mathcal{S}'(\mathbb{R}^{2d})$. Therefore

$$f_{\boldsymbol{\rho}_\circ} = \frac{1}{h^d}\,f_{\boldsymbol{\mu}_\circ} = \mathcal{F}_y\Big(\boldsymbol{\mu}_\circ\Big(x + \tfrac{hy}{2}, x - \tfrac{hy}{2}\Big)\Big) \underset{h\to 0}{\rightharpoonup} \rho_\circ(x)\,\delta_0(\xi)\,.$$

On the other side, in the case of pure states, writing $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\circ$ in the form

$$\boldsymbol{\rho} = |\psi\rangle\,\langle\psi|\,, \qquad\qquad \boldsymbol{\rho}_\circ = |\psi^\circ\rangle\,\langle\psi^\circ|$$

and noticing that

$$\tilde{f}_{|\psi\rangle\langle\psi|} = \tilde{f}_{|\psi^\circ\rangle\langle\psi^\circ|} + \tilde{f}_{|\psi-\psi^\circ\rangle\langle\psi-\psi^\circ|} + \tilde{f}_{|\psi^\circ\rangle\langle\psi-\psi^\circ|} + \tilde{f}_{|\psi-\psi^\circ\rangle\langle\psi^\circ|}$$

we deduce that

$$\tilde{f}_{\boldsymbol{\rho}} \geq \tilde{f}_{\boldsymbol{\rho}_\circ} + 2\,\mathrm{Re}\big(\tilde{f}_{|\psi^\circ\rangle\langle\psi-\psi^\circ|}\big)\,.$$

But now

$$\begin{aligned}\big\langle f_{|\psi^\circ\rangle\langle\phi|}, \varphi\big\rangle_{\mathcal{A}',\mathcal{A}} &= \iint_{\mathbb{R}^{2d}} \psi^\circ(x + \tfrac{hy}{2})\,\overline{\phi}(x - \tfrac{hy}{2})\,(\mathcal{F}_\xi\,\varphi)(x,y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \iint_{\mathbb{R}^{2d}} \overline{\phi}(x)\,\psi^\circ(x+hy)\;(\mathcal{F}_\xi\,\varphi)(x + \tfrac{hy}{2}, y)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

and this converges to 0 as ϕ converges weakly to 0. □

Examples of Wigner measures. As we saw in previous proof, a simple case where we can compute the Wigner measure is the case when $h^d\boldsymbol{\rho} = \boldsymbol{\mu}$ is an independent of $\hbar$ Hilbert–Schmidt operator (or more generally a compact sequence in L^2). Then $f_{\boldsymbol{\rho}} \rightharpoonup \mu$ with

$$\mu = \boldsymbol{\mu}(x,x)\,\delta_0(\xi)\,.$$

Another often used case is the case of **WKB approximations**. In this case, we take

$$\psi(x) = \varphi(x)\,e^{iS(x)/\hbar} \qquad \boldsymbol{\rho} = h^{-d}\left|\psi\right\rangle\left\langle\psi\right|$$

for some $\hbar$ independent real functions $\varphi \in L^2(\mathbb{R}^d)$ and $S \in W^{1,1}_{\mathrm{loc}}(\mathbb{R}^d)$. Then

$$\begin{aligned} f_{\boldsymbol{\rho}}(x,\xi) &= \int_{\mathbb{R}^d} e^{-2i\pi\,x\cdot\xi}\,\varphi(x+\tfrac{hy}{2})\,\overline{\varphi(x-\tfrac{hy}{2})}\,e^{\frac{i}{\hbar}\left(S(x+\frac{hy}{2})-S(x-\frac{hy}{2})\right)}\,\mathrm{d}y \\ &\underset{h\to 0}{\rightharpoonup} \left|\varphi(x)\right|^2\mathcal{F}_y\left(e^{2i\pi\,y\cdot\nabla S(x)}\right)(\xi) \end{aligned}$$

where the convergence holds in $\mathcal{S}'$, and so

$$\mu = \left|\varphi(x)\right|^2\delta_{\nabla S(x)}(\xi)\,.$$

Another typical example is the case of **coherent states** $\psi_{z_0} = \tau_{z_0}\psi_0$ with associated density matrix $\boldsymbol{\rho}_{z_0} = h^{-d}\left|\psi_{z_0}\right\rangle\left\langle\psi_{z_0}\right|$ already introduced before to build the Husimi transform. Then from Equation (24), we obtain $f_{\boldsymbol{\rho}_{z_0}} = g_h(z-z_0)$ that converges to a Dirac delta in the limit. Hence

$$\mu = \delta_{z_0} = \delta_{x_0}(x)\,\delta_{\xi_0}(\xi)\,.$$

One can similarly consider approaching a more general function (or measure) f of the phase space by doing a mixing of these coherent states

$$\tilde{\boldsymbol{\rho}}_f := \int_{\mathbb{R}^d} f(z)\,\boldsymbol{\rho}_z\,\mathrm{d}z\,.$$

Then the associated Wigner measure is $\mu = f$ since the Wigner transform is given by

$$f_{\tilde{\boldsymbol{\rho}}_f} = g_h * f \underset{h\to 0}{\to} f\,.$$

The above defined operator $\tilde{\boldsymbol{\rho}}_f$ is sometimes called the **(Anti-)Wick quantization**, or **Toeplitz operator**. From the definition we deduce that

$$f \geq 0 \implies \tilde{\boldsymbol{\rho}}_f \geq 0\,.$$

Denoting more generally the convolution by the Gaussian g_h by $\tilde{f} = g_h * f$ and its analogue operation on the operator side $\widetilde{\boldsymbol{\rho}} = \boldsymbol{\rho}_{g_h * f_{\boldsymbol{\rho}}}$, then we see that

$$\widetilde{f_{\boldsymbol{\rho}}} = \tilde{f}_{\boldsymbol{\rho}} = f_{\tilde{\boldsymbol{\rho}}} \qquad \tilde{f} = f_{\tilde{\boldsymbol{\rho}}_f} \qquad \widetilde{\boldsymbol{\rho}_f} = \boldsymbol{\rho}_{\tilde{f}} = \tilde{\boldsymbol{\rho}}_f \qquad \tilde{\boldsymbol{\rho}} = \boldsymbol{\rho}_{\tilde{f}_{\boldsymbol{\rho}}}\,.$$

4 The Vlasov–Poisson equation

We refer to [Gol13] for a nice exposition of the well-posedness and the regularity properties of the Vlasov–Poisson equation.

As seen in Section 2.2.2, for particles of mass $m = 1$ in dimension $d \geq 1$ with distribution $f = f(t, x, \xi) : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}_+$, one can write the Vlasov–Poisson equation in the form

$$\partial_t f + \xi \cdot \nabla_x f + E_f \cdot \nabla_\xi f = 0$$

where $E_f = E_f(t, x) = -\nabla V_f(t, x) = -\nabla K * \rho_f(t, x)$ is such that $-\Delta V_f = \rho_f$, where the convolution is with respect to x.

4.1 Conservation laws

The equation is a transport equation with divergence free field which, at least formally, conserves the positivity and the mass

$$M_0 = \int_{\mathbb{R}^d} \rho_f = \int_{\mathbb{R}^{2d}} f \, .$$

The fact that the underlying dynamics (i.e. the associated characteristics) preserve the Lebesgue measure also implies the conservation of the Casimir invariants $\int_{\mathbb{R}^{2d}} \Phi(f)$, such as the Lebesgue norms in the phase space $\|f\|_{L^p(\mathbb{R}^{2d})}$.

Conservation of energy. In the case when V is independent of f and t, that is $E(x) = -\nabla V(x)$ with V given, then defining

$$H = \frac{|\xi|^2}{2} + V(x)$$

one can write the equation as $\partial_t f = \{H, f\} = \nabla_x H \cdot \nabla_\xi f - \nabla_\xi H \cdot \nabla_x f$, and it follow from the chain rule that for any regular function $\phi = \Phi'$ that $\phi(H) \{H, f\} = \{\Phi(H), f\}$, so that, formally,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^{2d}} \phi(H) \, f = \int_{\mathbb{R}^{2d}} \{\Phi(H), f\} = 0 \, ,$$

that is, the quantities of the form $\int_{\mathbb{R}^{2d}} \phi(H) \, f$ are conserved. In particular, the total energy

$$\int_{\mathbb{R}^{2d}} H \, f = \int_{\mathbb{R}^{2d}} \frac{|\xi|^2}{2} f(t, x, \xi) \, \mathrm{d}x \, \mathrm{d}\xi + \int_{\mathbb{R}^d} \rho_f \, V$$

is conserved.

In the Vlasov–Poisson case, this is no longer the case since V_f is time dependent. One obtains instead that

$$\int_{\mathbb{R}^{2d}} \left(|\xi|^2 + V_f(x) \right) f(t, x, \xi) \, \mathrm{d}x \, \mathrm{d}\xi$$

is conserved.

Proof. Defining

$$H_f(x,\xi) := \frac{|\xi|^2}{2} + V_f(x)\,,$$

the previous computation and the fact that $\partial_t H_f = \partial_t V_f$ now gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2d}} H_f\, f = \int_{\mathbb{R}^{2d}} H_f\,\partial_t f + \partial_t H_f\, f = \int_{\mathbb{R}^{2d}} f\,\partial_t V_f\,. \tag{29}$$

But on the other hand, the symmetry in x and y in the integral

$$\int_{\mathbb{R}^{2d}} V_f\, f = \int_{\mathbb{R}^d} \rho_f\, K * \rho_f = \int_{\mathbb{R}^{2d}} K(x-y)\,\rho_f(x)\,\rho_f(y)\,\mathrm{d}x\,\mathrm{d}y$$

gives that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} \rho_f\, K * \rho_f = \int_{\mathbb{R}^d} \partial_t\rho_f\, K * \rho_f + \rho_f\, K * \partial_t\rho_f = 2\int_{\mathbb{R}^d} \rho_f\, K * \partial_t\rho_f$$

that is

$$\int_{\mathbb{R}^d} \rho_f\,\partial_t V_f = \frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} \rho_f\, V_f\,.$$

Hence finally, by Equation (29),

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2d}} \Big(|\xi|^2 + V_f(x)\Big)\, f(t,x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi = 2\,\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2d}} H_f\, f - \frac{1}{2}\,\rho_f\, V_f = 0\,.$$

□

4.2 Force field estimates

In dimension $d \neq 3$, the formula for the solution of the Poisson equation gives (choosing $K(x) \to 0$ when $x \to \infty$)

$$K(x) = \frac{C}{|x|^{d-2}}\,.$$

which is replaced by a logarithm if $d = 2$. In particular, $|\nabla K| \leq \frac{C}{|x|^{d-1}}$, and the Hardy–Littlewood–Sobolev inequality implies that if $(p,q) \in (1,\infty)^2$ are such that $\frac{1}{q} = \frac{1}{p} - \frac{1}{d}$, then there exists $C > 0$ such that for any $f \geq 0$,

$$\|E_f\|_{L^q} = \|\nabla K * \rho_f\|_{L^q} \leq C\,\|\rho_f\|_{L^p}\,.$$

One can also obtain estimates for $\nabla E_f = \nabla^2(-\Delta)^{-1}\rho_f$ from Calderón–Zygmund estimates (i.e. elliptic regularity) for $p \in (1,\infty)$,

$$\|\nabla E_f\|_{L^p} \leq C\,\|\rho_f\|_{L^p}\,.$$

To bound ρ_f in L^p norms, one can then use the decay in ξ together with the boundedness of f in $L^p(\mathbb{R}^{2d})$. The decay in ξ can be measured in terms of moments of f

$$M_n(f) := \int_{\mathbb{R}^{2d}} f\,|\xi|^n\,\mathrm{d}x\,\mathrm{d}\xi\,.$$

The boundedness of ρ_f in L^p is then a corollary of the following lemma, which can be found in [LP91].

Proposition 4.1 (Kinetic interpolation inequality)**.** *Let* $0 \leq k \leq n$ *and* $1 \leq p \leq r \leq \infty$ *be such that*

$$p' = \left(\tfrac{n}{k}\right)' \left(1 + \tfrac{d}{n}\right).$$

Then there exists $C > 0$ *such that for any* $f \geq 0$,

$$\left\| \int_{\mathbb{R}^d} f\, |\xi|^k \,\mathrm{d}\xi \right\|_{L^p} \leq C\, \|f\|_{L^r(\mathbb{R}^{2d})}^{\theta}\, M_n(f)^{1-\theta},$$

where $\theta = r'/p'$.

Remark 4.2.1. In particular, taking $k = 0$ and $r = \infty$, one deduces that

$$\|\rho_f\|_{L^p} \leq C\, \|f\|_{L^\infty(\mathbb{R}^{2d})}^{1/p'}\, M_n(f)^{1/p}$$

with $p' = 1 + \frac{d}{n}$, i.e. $p = 1 + \frac{n}{d}$.

Proof of Lemma 4.1. Up to replacing f by $f\,|\xi|^k$ and $|\xi|^n$ by $|\xi|^{n-k}$, one can assume that $k = 0$. Let $R > 0$. Then by Hölder's inequality

$$\int_{|\xi| \leq R} f \,\mathrm{d}\xi \leq \|f\|_{L^r_\xi}\, |\{\, |\xi| \leq R \,\}|^{1/r'} = C\, \|f\|_{L^r_\xi}\, R^{d/r'}$$

where $C = \left(\frac{\omega_d}{d}\right)^{1/r'}$ with $\omega_d = \frac{2\,\pi^{d/2}}{\Gamma(d/2)}$ the size of the unit ball in $\mathbb{R}^d$. On the other side,

$$\int_{|\xi| \geq R} f \,\mathrm{d}\xi \leq R^{-n} \int_{|\xi| \geq R} f\, |\xi|^n \,\mathrm{d}\xi \leq R^{-n} \int_{\mathbb{R}^d} f\, |\xi|^n \,\mathrm{d}\xi\,.$$

Optimizing the sum of the right-hand side of these two inequalities with respect to R leads to take $R^{n+d/r'} = \frac{n\,r'}{d\,C}\, \|f\|_{L^r_\xi}^{-1} \int_{\mathbb{R}^d} f\, |\xi|^n \,\mathrm{d}\xi$. Noticing that $\frac{n\,r'}{d} = \frac{\theta}{1-\theta}$, it yields

$$\rho_f(x) \leq C_\theta \left(C\, \|f\|_{L^r_\xi} \right)^{\theta} \left(\int_{\mathbb{R}^d} f\, |\xi|^n \,\mathrm{d}\xi \right)^{1-\theta}$$

where $C_\theta = \left(\frac{\theta}{1-\theta}\right)^{1-\theta} + \left(\frac{1-\theta}{\theta}\right)^{\theta} = \frac{1}{\theta^\theta\,(1-\theta)^{1-\theta}}$. Therefore, taking the power p, integrating in x and then noticing that $\theta = \frac{r'}{p'} \iff \frac{p\theta}{r} + p\,(1-\theta) = 1$ to use Hölder's inequality, we obtain

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_f^p &\leq C_\theta^p \int_{\mathbb{R}^d} \left(C^r\, \|f\|_{L^r_\xi}^r \right)^{\frac{p\theta}{r}} \left(\int_{\mathbb{R}^d} f\, |\xi|^n \,\mathrm{d}\xi \right)^{p(1-\theta)} \mathrm{d}x \\ &\leq C_\theta^p\, C^{p\theta}\, \|f\|_{L^r(\mathbb{R}^{2d})}^{p\theta} \left(\iint_{\mathbb{R}^{2d}} f\, |\xi|^n \,\mathrm{d}x \,\mathrm{d}\xi \right)^{p(1-\theta)} \end{aligned}$$

which proves the claimed inequality with $C = \theta^{-\theta}\,(1-\theta)^{\theta-1} \left(\frac{\omega_d}{d}\right)^{1/p'}$. □

4.3 Propagation of moments

Moments of order 2 are bounded thanks to the conservation of energy and the fact that one can bound the potential energy by the kinetic energy using the Hardy–Littlewood–Sobolev and the Kinetic interpolation inequalities.

In dimension $d = 2$, one obtains using the estimates of the previous section,

$$\partial_t M_n(f) \leq C \, \|f\|_{L^\infty}^{1/2} \, M_0^{1/2} M_n(f)$$

which implies the global propagation of moments by the Grönwall lemma, that is

$$M_n(f) \leq M_n(f^{\mathrm{in}}) \, e^{C\|f\|_{L^\infty}^{1/2} M_0^{1/2} t}.$$

In dimension $d = 3$, it is not difficult to obtain in the same way propagation of moments up to some maximal time T. Global in time estimates are possible and were proved in [LP91].

5 Trace Inequalities

5.1 Correspondence principle

5.1.1 Motivation

The quantum analogue of the Vlasov equation is the Hartree equation

$$i\hbar \, \partial_t \boldsymbol{\rho} = [H_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \tag{30}$$

where $H_{\boldsymbol{\rho}} = \frac{|\boldsymbol{p}|^2}{2} + V_{\boldsymbol{\rho}}$ with $V_{\boldsymbol{\rho}}$ the operator of multiplication by the function $V_{\boldsymbol{\rho}}(x) = K * \rho_{\boldsymbol{\rho}}(x)$.

To prove that solutions of the Hartree equation converge to solutions of the Vlasov equation when $\hbar \to 0$, our strategy will be to mimic proofs of uniqueness/stability of the Vlasov equation, and try to translate them to the quantum setting. As seen in the previous section, this needs however to obtain regularity estimates uniform in $\hbar$.

One could try to use the Wigner equation. However, L^p norms of the Wigner transform with $p \neq 2$ are not conserved quantities of the Wigner equation. Moreover, it is not true that the Wigner transform of a positive operator is positive, and not true that the Wigner transform of a trace class operator is in L^1.

Instead, one observes that if $\boldsymbol{\rho} = \boldsymbol{\rho}(t)$ is a solution of the Hartree equation (30) with initial condition $\boldsymbol{\rho}(0) = \boldsymbol{\rho}^{\mathrm{in}}$, then for any $n \in \mathbb{N}$, at least formally, $i\hbar \, \partial_t \boldsymbol{\rho}^n = [H_{\boldsymbol{\rho}}, \boldsymbol{\rho}^n]$. More generally, one can prove that the Schrödinger equation $i\hbar \, \partial_t \boldsymbol{\rho} = H_{\boldsymbol{\rho}} \psi$ can be written in terms of a unitary operator U_t, i.e. $\psi(t, x) = U_t \psi(0, x)$, from which is follows that $\boldsymbol{\rho}$ can be written

$$\boldsymbol{\rho} = U_t^* \, \boldsymbol{\rho} \, U_t \, ,$$

from which it follows that Equation (30) preserves the positivity and the Schatten norms (as we will see in Section 5.4). Hence we will rather work directly with Equation (30), traces and operators, and reason by analogy.

5.1.2 The Quantum–Classical dictionary

Correspondence principle in our setting.

1. The phase space coordinates x and ξ are associated to the operators x (of multiplication by x) and $\boldsymbol{p} = -i\hbar\nabla$, and, more generally, functions on the phase space (observables or densities) are associated to operators on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C})$.

2. The scaled diagonal of the kernel of an operator A (i.e. $h^d A(x,x)$) corresponds to the integral with respect to the momentum.

3. The scaled commutators of operators A and B (i.e. $\frac{1}{i\hbar}[A,B]$) associated to the functions of the phase space f and g are associated to the Poisson brackets $\{g,f\} = \nabla_x g \cdot \nabla_\xi f - \nabla_\xi g \cdot \nabla_x f$

This gives the following dictionary.

	Classical	**Quantum**
Phase space	$z = (x,\xi) \in \mathbb{R}^{2d}$	$\mathbf{z} = (x, \boldsymbol{p}) = (x, -i\hbar\nabla) \in \mathcal{L}(\mathcal{H})^2$
Distribution	$f \in \mathcal{M}(\mathbb{R}^{2d})$	$\boldsymbol{\rho} \in \mathcal{L}^1(\mathcal{H})$
Density	$\rho_f = \int_{\mathbb{R}^d} f \,\mathrm{d}\xi$	$\rho_{\boldsymbol{\rho}} = h^d \,\boldsymbol{\rho}(x,x)$
Expectation	$\langle g\rangle_f = \int_{\mathbb{R}^{2d}} g\, f \,\mathrm{d}x\,\mathrm{d}\xi$	$\langle A\rangle_{\boldsymbol{\rho}} = h^d \operatorname{Tr}(A\,\boldsymbol{\rho})$
Kinetic energy	$\frac{1}{2}\int_{\mathbb{R}^{2d}} \lvert\xi\rvert^2 \, f\,\mathrm{d}x\,\mathrm{d}\xi$	$\frac{h^d}{2}\operatorname{Tr}\Big(\lvert\boldsymbol{p}\rvert^2\,\boldsymbol{\rho}\Big) = -\frac{h^d}{2}\operatorname{Tr}\big(\hbar^2\Delta\,\boldsymbol{\rho}\big)$
Hamiltonian	$H_f(x,\xi) = \frac{\lvert\xi\rvert^2}{2} + V_f(x)$	$H_{\boldsymbol{\rho}} = \frac{\lvert\boldsymbol{p}\rvert^2}{2} + V_{\boldsymbol{\rho}}(x)$
Dynamics	Vlasov	Hartree
(mean-field)	$\partial_t f = \{H_f,\, f\}$	$i\hbar\,\partial_t\boldsymbol{\rho} = [H_{\boldsymbol{\rho}}, \boldsymbol{\rho}]$
Shift	$f(z-z_0) = f(x-x_0, \xi-\xi_0)$	$\mathsf{T}_{z_0}\boldsymbol{\rho} = \tau_{z_0}\,\boldsymbol{\rho}\,\tau_{z_0}^*, \tau_{z_0} = e^{i(\xi_0\cdot x - x_0\cdot\boldsymbol{p})/\hbar}$
Gradients	$\nabla_x f = \{-v, f\},\ \nabla_\xi f = \{x, f\}$	$\boldsymbol{\nabla}_x\boldsymbol{\rho} = [\nabla, \boldsymbol{\rho}]\,,\ \boldsymbol{\nabla}_\xi\boldsymbol{\rho} = \left[\frac{x}{i\hbar}, \boldsymbol{\rho}\right]$
Norms	Lebesgue	Schatten
	$\lVert f\rVert_{L^p(\mathbb{R}^{2d})}$	$\lVert\boldsymbol{\rho}\rVert_{\mathcal{L}^p} = h^{\frac{d}{p}}\operatorname{Tr}(\lvert\boldsymbol{\rho}\rvert^p)^{\frac{1}{p}}$
	Sobolev	Sobolev
	$\lVert\nabla f\rVert_{L^p(\mathbb{R}^{2d})}$	$\lVert\boldsymbol{\nabla}\boldsymbol{\rho}\rVert_{\mathcal{L}^p} = \Big\lVert \lvert\boldsymbol{\nabla}_x\boldsymbol{\rho}\rvert^2 + \lvert\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\rvert^2 \Big\rVert_{\mathcal{L}^{\frac{p}{2}}}^{1/2}$

The product of convolution being bilinear, there is no unique choice in the quantum case. However there are choices with good properties if one mixes operators and functions (see e.g. [Wer84, Laf24]).

- Operator-valued convolution of an operator and a function:

$$f \star \boldsymbol{\rho} = \int_{\mathbb{R}^{2d}} f(z)\,\mathsf{T}_z\boldsymbol{\rho}\,\mathrm{d}z\,.$$

- Function-valued convolution of two operators:

$$(\boldsymbol{\rho} * \boldsymbol{\mu})(z) := (f_{\boldsymbol{\mu}} * f_{\boldsymbol{\rho}})\,(z) = h^d \operatorname{Tr}\Big(\boldsymbol{\rho}\,\mathsf{T}_z\boldsymbol{\mu}^{(-)}\Big)\,,$$

  where $\boldsymbol{\mu}^{(-)}(x,y) = \boldsymbol{\mu}(-x,-y)$, i.e. $f_{\boldsymbol{\mu}^{(-)}}(z) = f_{\boldsymbol{\mu}}(-z)$.

Similarly, for the Fourier transform, according to formulas (11) and (22), one obtains the following.

- Function-valued Fourier transform of an operator:

$$\widehat{f_{\boldsymbol{\rho}}}(z) = h^d \operatorname{Tr}\big(e^{-2i\pi\, z\cdot \mathbf{z}}\, \boldsymbol{\rho}\big)\,.$$

- Operator-valued Fourier transform of a function:

$$\boldsymbol{\rho}_{\widehat{f}} = \int_{\mathbb{R}^{2d}} f(z)\, e^{-2i\pi\, z\cdot \mathbf{z}}\, \mathrm{d}z\,.$$

The above transformations are $L^2-\mathcal{L}^2$ isometries, and verify analogues of the Hausdorff–Young inequality: if $p \in [1,2]$, then $\|\widehat{f_{\boldsymbol{\rho}}}\|_{L^{p'}} \leq \|\boldsymbol{\rho}\|_{\mathcal{L}^p}$ and $\|\boldsymbol{\rho}_{\widehat{f}}\|_{\mathcal{L}^{p'}} \leq \|\boldsymbol{\rho}\|_{L^p}$. One could define an operator-valued Fourier transform of an operator as $\widehat{\boldsymbol{\rho}} = \boldsymbol{\rho}_{\widehat{f_{\boldsymbol{\rho}}}}$, which would still be an isometry on $\mathcal{L}^2$, but it is not clear it would verify Hausdorff–Young-like inequalities.

5.2 Decomposition of bounded operators

Proposition 5.1. *Let $A \in \mathcal{L}^\infty$ satisfy $A \geq 0$. Then there exists a unique $B \in \mathcal{L}^\infty$ with $B \geq 0$ such that $B^2 = A$. Furthermore, B commutes with every bounded operator which commutes with A.*

Therefore, for any $A \in \mathcal{L}^\infty$, since $A^*A \geq 0$, we can define

$$|A| := \sqrt{A^*A}.$$

Remark 5.2.1. Warning about the fact that it is in general not true that $|AB| = |A|\,|B|$, $|A^*| = |A|$ or $|A+B| \leq |A| + |B|$. However $|\lambda A| = |\lambda|\,|A|$. Notice also that $|AB| = ||A|\,B|$. In particular, if $U \in \mathcal{I}$, then $|UA| = |A|$.

Proof of Proposition 5.1. Let us prove the existence first. Up to multipying A by a positive constant, it is sufficient to look at the case when $\|A\|_\infty \leq 1$. Then $\|1-A\|_\infty = \sup_\varphi \langle\varphi\,|\,(1-A)\,\varphi\rangle \leq 1$. Hence, using the fact that for any $|z| \leq 1$, the series

$$\sqrt{1-z} = \sum_{n=0}^{\infty} \binom{1/2}{n} (-1)^n\, z^n$$

converges absolutely, we deduce that the series $\sum \binom{1/2}{n} (-1)^n\,(1-A)^n$ converges in operator norm to a positive operator $B \in \mathcal{L}^\infty$. Moreover, since the convergence is absolute, we can square the series $\sum \binom{1/2}{n} (-1)^n\,(1-A)^n$ and rearrange the terms to get that $B^2 = A$.

We now prove the uniqueness. If $D \geq 0$ also satisfies $D^2 = A$, then noticing that $D\,A = D^3 = A\,D$, one deduces that D commutes with A and B. Therefore,

$$(B-D)\,B\,(B-D) + (B-D)\,D\,(B-D) = \big(B^2 - D^2\big)\,(B-D) = 0$$

and since both terms in the right-hand side are positive, they are zero, and so their difference $(B-D)^3 = 0$. As $B-D$ is self adjoint, we finally get $\|B-D\|_\infty^4 = \|(B-D)^4\|_\infty = 0$. ☐

The following decomposition is the equivalent of the decomposition $z = |z|\,e^{i\theta}$ for complex numbers.

Theorem 5.2 (Polar decomposition)**.** *Let $A \in \mathcal{L}^\infty$. Then there exists an operator U satisfying $U_{|\operatorname{Ker} A} = 0$, $U_{|(\operatorname{Ker} A)^\perp} = U_{|\overline{\operatorname{Ran} A}}$ is an isometry and*

$$A = U\,|A|$$

or equivalently $|A| = U^* A$.

One takes $U_{|\operatorname{Ran}(|A|)}(|A|\,\psi) = A\psi$.

Since we know how to diagonalize positive compact operators, we will use the above theorem to get another decomposition for general compact operators.

Theorem 5.3 (Singular value decomposition)**.** *Let $A \in \mathcal{L}^\infty$, then there exists a unique family $(\mu_j(A))_{j\in J}$ with $J \subseteq \mathbb{N}$ satisfying $\mu_0(A) \geq \mu_1(A) \geq \cdots > 0$ called the **singular values** of A such that*

$$A = \sum_{j\in J} \mu_j(A)\,|\phi_j\rangle\,\langle\psi_j| \tag{31}$$

where $(\phi_j)_{j\in J}$ and $(\psi_j)_{j\in J}$ are orthonormal sets.

Proof. By Theorem 1.1, since $|A| = U^*A \geq 0$ is a compact self-adjoint operator, it can be written in the form

$$|A| = \sum_{j\in J} \mu_j(A)\,|\psi_j\rangle\,\langle\psi_j|$$

and so since $A = U\,|A|$, we can write it under the form (31) where $\phi_j := U\phi_j$ is also an orthonormal family because U is an isometry on $(\operatorname{Ker}(A))^\perp = \operatorname{Ran}|A|$. Uniqueness follows from the fact that Equation (31) implies that $\mu_j(A)^2$ are the non-zero eigenvalues of A^*A. ☐

5.3 Singular values

If $A \in \mathcal{K}$, we define $(\lambda_j(A))_{j\geq 0}$ its eigenvalues ordered so that $|\lambda_0| \geq |\lambda_1| \geq \ldots$. As seen in the proof above, the singular values $(\mu_j(A))_{j\geq 0}$ as just the ordered eigenvalues of $|A|$, so $\mu_j(A) = \lambda_j(|A|)$. More generally, $\mu_j(A)^p = \lambda_j(|A|)^p = \lambda_j(|A|^p) = \mu_j(|A|^p)$. Note that

$$\mu_0(A) = \lambda_0(|A|) = \|A\|_\infty = |\lambda_0(A)|\,.$$

It also follows from (31) that

$$\mu_j(A) = \mu_j(A^*) \tag{32}$$

In particular, for unitary operators

$$\mu_j(UA) = \mu_j(A) = \mu_j(AU)$$

where the last identity comes from the fact that $\mu_j(AU) = \mu_j(U^*A^*) = \mu_j(A^*)$.

Min-Max formula. The min-max characterization of eigenvalues can be written for compact operators as follows

$$\lambda_j(A) = \min_{\substack{X\subset\mathcal{H}\\ \dim X = j}} \max_{\substack{\varphi\in X^\perp\\ \|\varphi\|_{\mathcal{H}}=1}} \langle \varphi \,|\, A\varphi \rangle\,.$$

Since $\langle \varphi \,|\, A^*A\varphi \rangle = \|A\varphi\|_{\mathcal{H}}^2$ and $\mu_j(A)^2 = \lambda_j(|A|^2)$, we deduce the following min-max characterization of the singular eigenvalues

$$\mu_j(A) = \min_{\substack{X\subset\mathcal{H}\\ \dim X = j}} \max_{\substack{\varphi\in X^\perp\\ \|\varphi\|_{\mathcal{H}}=1}} \|A\varphi\|_{\mathcal{H}}\,. \tag{33}$$

These formulas are useful to obtain inequalities involving eigenvalues. In particular, the following inequalities hold.

Proposition 5.4. *Let A and B be compact operators. Then for any $(j,k)\in\mathbb{N}_0^2$,*

$$\mu_j(BA) \le \|B\|_\infty\, \mu_j(A) \tag{34}$$

$$\mu_j(AB) \le \|B\|_\infty\, \mu_j(A) \tag{35}$$

$$\mu_{j+k}(A+B) \le \mu_j(A) + \mu_k(B) \qquad \textit{(See Fan [Fan51])} \tag{36}$$

Remark 5.3.1. The same inequality also holds with the sum replaced by a product (See [Fan51]).

Remark 5.3.2. In general, $\mu_j(AB)\neq\mu_j(BA)$. This is not the case for the spectrum which satisfies $\sigma(AB)\setminus\{0\} = \sigma(BA)\setminus\{0\}$ (See [Dei78]). Intuitively, if A and B are matrices with A invertible, then $BA = A^{-1}(AB)A$ is similar to AB and so if $AB\varphi = \lambda\varphi$, then $BA(A^{-1}\varphi) = \lambda(A^{-1}\varphi)$.

Proof. Inequality (34) follows from the min-max Formula (33) and the fact that $\|BA\varphi\|_{\mathcal{H}} \le \|B\|_{\mathcal{H}}\,\|A\varphi\|_{\mathcal{H}}$. Inequality (35) then follows from Inequality (34) and the adjoint formula (32) since

$$\mu_j(AB) = \mu_j(B^*A^*) \le \|B^*\|_\infty\,\mu_j(A^*) = \|B\|_\infty\,\mu_j(A)\,.$$

Define $Q_A(\psi_1,\dots,\psi_j) := \max\{\, \|A\varphi\|_{\mathcal{H}} : \|\varphi\|_{\mathcal{H}} = 1, \varphi\in\{\,\psi_1,\dots,\psi_j\,\}^\perp \,\}$, so that the j-th eigenvalue of A is the minimum of Q_A over all families of $\{\,\psi_1,\dots,\psi_j\,\}$. Then the triangle inequality and the definition of the maximum imply that

$$\begin{aligned} Q_{A+B}(\psi_1,\dots,\psi_{j+k}) &\le Q_A(\psi_1,\dots,\psi_{j+k}) + Q_B(\psi_1,\dots,\psi_{j+k}) \\ &\le Q_A(\psi_1,\dots,\psi_j) + Q_B(\psi_{j+1},\dots,\psi_{j+k})\,. \end{aligned}$$

The last inequality (36) then follows by the min-max principle. □

5.4 Schatten spaces and Trace

5.4.1 Schatten spaces

The Schatten spaces are defined for $p\in[1,\infty]$ by $\mathfrak{S}^p = \{\, A\in\mathcal{K} : \|A\|_p < \infty \,\}$ where the Schatten norms are

$$\|A\|_p = \|(\mu_j(A))_{j\ge0}\|_{\ell^p} = \left(\sum_{j=0}^{\infty}\mu_j(A)^p\right)^{1/p}.$$

From the above considerations on singular values we deduce that if U is unitary and $r \geq 1$,

$$\begin{aligned} \|A\|_p &= \|A^*\|_p\,, & \||A|\|_p &= \|A\|_p \\ \||A|^r\|_p &= \|A\|_{rp}^r\,, & \|A\|_p &= \|AU\|_p = \|UA\|_p \\ \|AB\|_p &\leq \|A\|_p\,\|B\|_\infty\,, & \|AB\|_p &\leq \|A\|_\infty\,\|B\|_p\,. \end{aligned}$$

and so the Schatten classes are two-sided ideals of bounded operators.

Operators in $\mathfrak{S}^\infty$ are just the compact operators and operators in $\mathfrak{S}^1$ are called trace class operators. We can check that the definition of the 2-Schatten norm correspond with the one given for the Hilbert–Schmidt norm given in (3), since doing the singular value decomposition of A in the form (31) yields $A\psi_j = \mu_j(A)\,\phi_j$, and so

$$\|A\|_2^2 = \sum_{j\geq 0} \mu_j(A)^2 = \sum_{j\geq 0} \|A\psi_j\|_{\mathcal{H}}^2 = \sum_{j,k\geq 0} |\langle \phi_k \,|\, A\psi_j\rangle|^2 \tag{37}$$

the last equality following from the Parseval identity. In particular, if $A \in \mathcal{K}_+$, then replacing A by $\sqrt{A}$ in the above formula shows that

$$\|A\|_1 = \big\|\sqrt{A}\big\|_2^2 = \sum_{j\geq 0} \big\|\sqrt{A}\psi_j\big\|_{\mathcal{H}}^2 = \sum_{j\geq 0} \langle \psi_j \,|\, A\psi_j\rangle = \mathrm{Tr}(A)\,. \tag{38}$$

To get an explicit formula of the trace norm of an operator in term of its integral kernel is in general not easy. For Hilbert–Schmidt operators, a necessary and sufficient condition can be given in terms of the maximal function MK_A of the kernel of A. If $A \in \mathfrak{S}^2$, then (see e.g. [Sim05, Theorem A.3])

$$A \in \mathfrak{S}^1 \iff \int_{\mathbb{R}^d} (MK_A)(x,x)\,\mathrm{d}x < \infty\,.$$

5.4.2 Trace

The space $\mathfrak{S}^1$ of trace class operators offers a good framework to define the trace. More precisely, if $A \in \mathfrak{S}^1$ is in the singular value form (31), then for any φ_j orthonormal basis

$$\mathrm{Tr}(A) := \sum_{j\geq 0} \langle \varphi_j | A\varphi_j\rangle = \sum_{j\geq 0} \mu_j(A)\,\langle \psi_j | \phi_j\rangle \tag{39}$$

is independent of the basis. Moreover, the sums above converge absolutely and

$$|\mathrm{Tr}(A)| \leq \|A\|_1\,. \tag{40}$$

Proof of (39) *and* (40). Notice that by the Parseval identity, for any $j \in \mathbb{N}$,

$$\sum_{n\in\mathbb{N}} |\langle \varphi_n \,|\, \phi_j\rangle|^2 = \|\phi_j\|_{L^2}^2 = 1\,.$$

Thus, by the Cauchy–Schwarz inequality

$$\sum_{j,n} |\mu_j(A)\ \langle \varphi_n \,|\, \phi_j\rangle\,\langle \psi_j \,|\, \varphi_n\rangle| \leq \sum_j \mu_j(A) = \|A\|_1\,.$$

Therefore, we can interchange the order of the sums in the following double sum

$$\sum_n \langle \varphi_n \,|\, A\,\varphi_n\rangle = \sum_j \mu_j(A)\,\langle \psi_j | \sum_n |\varphi_n\rangle\,\langle \varphi_n \,|\, \phi_j\rangle = \sum_j \mu_j(A)\,\langle \psi_j \,|\, \phi_j\rangle$$

which gives the result. □

From the previously shown Formula (38) and the fact that $\mu_j(A)^p = \mu_j(|A|^p)$, we see that we can write the Schatten norms using the trace by writing that for any $p \in [1,\infty)$,

$$\|A\|_p^p = \mathrm{Tr}(|A|^p)\,.$$

As seen in Section 3.2, multiplying the trace by h^d gives the analogue of the integral on the phase space of classical statistical mechanics. With this in mind, we define the quantum analogue of the Lebesgue norms in the phase space by the following scaled Schatten norms

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} := h^{\frac{d}{p}}\,\|\boldsymbol{\rho}\|_p = \left(h^d\,\mathrm{Tr}(|\boldsymbol{\rho}|^p)\right)^{\frac{1}{p}}\,. \tag{41}$$

The following natural formulas are, surprisingly, difficult to prove (See [Sim05, Equations (3.2) and (3.3)]).

Theorem 5.5 (Carleman)**.** *Let $A \in \mathfrak{S}^2$. Then*

$$\mathrm{Tr}\big(A^2\big) = \sum_{j\in J} \lambda_j(A^2)\,.$$

Theorem 5.6 (Lidskii)**.** *Let $A \in \mathfrak{S}^1$. Then*

$$\mathrm{Tr}(A) = \sum_{j\in J} \lambda_j(A)\,. \tag{42}$$

Cyclicity of the trace. One of the good properties of the trace that generalizes to trace class operators is the cyclicity property

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA)\,. \tag{43}$$

However notice that it is false in general that for any operator $A, B \in \mathcal{L}(\mathcal{H})$, $\mathrm{Tr}([A,B]) = 0$, since for instance $\left[x_j, \boldsymbol{p}_j\right] = i\hbar$ is a multiple of the identity on L^2 and so has undefined (or at least infinite) trace.

Proposition 5.7 (Commutation in the trace)**.** *Equation (43) holds if*

1. *$(A,B) \in (\mathcal{L}^\infty)^2$ are such that $AB \in \mathfrak{S}^1$ and $BA \in \mathfrak{S}^1$.*
2. *$(A,B) \in \mathcal{L} \times \mathcal{K}$ are such that $AB \in \mathfrak{S}^1$ and $BA \in \mathfrak{S}^1$.*
3. *$(A,B) \in \mathcal{L} \times \mathcal{K}$ are self-adjoint, A is densely defined and such that $AB \in \mathfrak{S}^1$ or $BA \in \mathfrak{S}^1$.*

Proof.

1. The first inequality follows from Lidskii's formula (42) and the fact that the eigenvalues of AB and BA are the same. See [Sim05, Corollary 3.8].

2. Write $B = \sum_j \mu_j(B)\,|\phi_j\rangle\,\langle\psi_j|$. Then by Formula (39) for the trace

$$\mathrm{Tr}(AB) = \sum_n \langle\psi_n\,|\,AB\,\psi_n\rangle = \sum_n\sum_j \mu_j(B)\,\langle\psi_n\,|\,A\,\phi_j\rangle\,\langle\psi_j\,|\,\psi_n\rangle$$
$$= \sum_n \mu_n(B)\,\langle\psi_n\,|\,A\,\phi_n\rangle = \sum_n \langle\phi_n\,|\,BA\,\phi_n\rangle = \mathrm{Tr}(BA)\,.$$

3. If $A \in \mathcal{L}$ is densely defined and $B \in \mathcal{L}^\infty$, then $(BA)^* = A^*B^*$. Hence since the singular values are invariant by taking the adjoint $\mathrm{Tr}(|AB|) = \mathrm{Tr}(|BA|) < \infty$ and so Criterion 3 follows from Criterion 2. □

In some cases, when dealing with an unbounded operator A and a nice operator B, one wants to think of $\mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B})$ as the correct meaning of $\mathrm{Tr}(AB)$. For instance, if $A = \Delta$ and $\boldsymbol{\rho} = |\psi\rangle\,\langle\psi|$ with $\psi \in H^n$, then there is no problem to define $\mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B}) = \langle\psi\,|\,\Delta\psi\rangle = -\|\nabla\psi\|_{L^2}$ if $n \geq 1$. On the other hand, $BA = \psi\,\langle\psi\,|\,\Delta\,\cdot\rangle = |\psi\rangle\,\langle\Delta\psi|$ is only a well defined operator on L^2 if $n \geq 2$. In this latter case, $\mathrm{Tr}(BA) = \langle\Delta\psi\,|\,\psi\rangle = \mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B})$.

Proposition 5.8. *Let $A \in \mathcal{L}$ be a densely defined operator and $B \in \mathcal{L}^\infty$. Then if $B \in \mathcal{K}_+$ and ($\sqrt{B}\,A\,\sqrt{B} \in \mathfrak{S}^1$ or $A \geq 0$) then*

$$\mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B}) = \mathrm{Tr}(AB) \qquad \text{if } AB \in \mathfrak{S}^1 \tag{44}$$

$$\mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B}) = \mathrm{Tr}(BA) \qquad \text{if } BA \in \mathfrak{S}^1 \tag{45}$$

If $(A, B) \in \mathcal{L}_+ \times \mathcal{K}$ are such that $\sqrt{A}\,B\,\sqrt{A} \in \mathfrak{S}^1$, $\sqrt{A}\,\sqrt{|B|} \in \mathfrak{S}^2$ and $\sqrt{A}\,\sqrt{|B^*|} \in \mathfrak{S}^2$, then

$$\mathrm{Tr}(\sqrt{A}\,B\,\sqrt{A}) = \mathrm{Tr}(AB) \qquad \text{if } AB \in \mathfrak{S}^1 \tag{46}$$

$$\mathrm{Tr}(\sqrt{A}\,B\,\sqrt{A}) = \mathrm{Tr}(BA) \qquad \text{if } BA \in \mathfrak{S}^1 \tag{47}$$

$$\mathrm{Tr}(\sqrt{A}\,B\,\sqrt{A}) = \mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B}) \qquad \text{if } B \geq 0 \tag{48}$$

If $(A, B) \in \mathcal{L}_+ \times \mathcal{L}_+^\infty$ are such that $\sqrt{A}\sqrt{B} \in \mathfrak{S}^2$ and A is densely defined, then

$$\mathrm{Tr}(\sqrt{B}\,A\sqrt{B}) = \mathrm{Tr}(\sqrt{A}\,B\sqrt{A}) \tag{49}$$

Proof of (44) *and* (45). Since $B \geq 0$, we can write $B = \sum_j \mu_j(B)\,|\psi_j\rangle\,\langle\psi_j|$. Then by (39)

$$\begin{aligned}\mathrm{Tr}(\sqrt{B}\,A\,\sqrt{B}) &= \sum_n \sum_{j,k} \sqrt{\mu_j(B)\mu_k(B)}\,\langle\psi_n\,|\,\psi_j\rangle\,\langle\psi_j\,|\,A\,\psi_k\rangle\,\langle\psi_k\,|\,\psi_n\rangle \\ &= \sum_n \mu_n(B)\,\langle\psi_n\,|\,A\,\psi_n\rangle\end{aligned}$$

and we conclude as in the proof of 2.

If $A \geq 0$ and $AB \in \mathfrak{S}^1$ or $BA \in \mathfrak{S}^1$, then $\sqrt{B}\,A\sqrt{B} = |\sqrt{A}\sqrt{B}|^2 \in \mathcal{L}^1$ by the Araki–Lieb–Thirring inequality (which we will prove later, see Inequality (5.17)), so this reduces to the first case. ☐

Proof of (46). Since $B \in \mathcal{K}$, we can write $B = \sum_j \mu_j(B)\,|\phi_j\rangle\,\langle\psi_j|$. Notice that by the Cauchy–Schwarz inequality and Plancherel identity

$$\begin{aligned}\sum_{n,j} \left|\mu_j(B)\,\left\langle\psi_n\,\middle|\,\sqrt{A}\,\phi_j\right\rangle\left\langle\psi_j\,\middle|\,\sqrt{A}\,\psi_n\right\rangle\right| &\leq \sum_j \mu_j(B)\,\left\|\sqrt{A}\,\phi_j\right\|_{L^2}\left\|\sqrt{A}\,\psi_j\right\|_{L^2} \\ &\leq \left(\sum_j \mu_j(B)\,\left\langle\phi_j\,\middle|\,\sqrt{A}\,\phi_j\right\rangle\right)^{1/2}\left(\sum_j \mu_j(B)\,\left\langle\psi_j\,\middle|\,\sqrt{A}\,\psi_j\right\rangle\right)^{1/2} \\ &\leq \mathrm{Tr}(\sqrt{|B^*|}A\sqrt{|B^*|})^{1/2}\,\mathrm{Tr}(\sqrt{|B|}A\sqrt{|B|})^{1/2}\end{aligned}$$

where the last inequality follows from the proof of (44). Hence, since $A \geq 0$, the double sum is absolutely convergent if $\sqrt{A}\sqrt{|B^*|} \in \mathfrak{S}^2$ and $\sqrt{A}\sqrt{|B|} \in \mathfrak{S}^2$, in which case

$$\mathrm{Tr}(\sqrt{A}\,B\,\sqrt{A}) = \sum_j \mu_j(B)\,\langle\psi_j\,|\,A\,\phi_j\rangle$$

and we conclude as in the proof of (45). ☐

Proof of (49). If $A \in \mathcal{L}$ is densely defined and $B \in \mathcal{L}^\infty$, then $(\sqrt{B}\sqrt{A})^* = \sqrt{A}\sqrt{B}$. Hence since the singular values are invariant by taking the adjoint $\|\sqrt{A}\sqrt{B}\|_2 = \|\sqrt{B}\sqrt{A}\|_2$. ☐

5.4.3 Weak Schatten spaces

In the same way as the Schatten norms are the analogue of the Lebesgue norms, the quantum analogue of the Lorentz spaces $L^{p,q}$ (the spaces obtained by real interpolation of Lebesgue spaces) can be defined following Birman–Solomyak [BS77] for any $(p,q) \in (0,\infty]^2$ by

$$\mathfrak{S}^{p,q} = \left\{A \in \mathcal{K},\ \left\| j^{\frac{1}{p}-\frac{1}{q}}\, \mu_j(A)\right\|_q < \infty\right\}.$$

Similarly as for Lorentz spaces, $\mathfrak{S}^{p,p} = \mathfrak{S}^p$ and defining $\tilde{\mu}_j(A) = \frac{1}{j}\sum_{k=0}^{j} \mu_k(A)$, then a norm on the space $\mathfrak{S}^{p,q}$ is given for $p > 1$ and $q \geq 1$ by

$$\|A\|_{p,q} = \left\| j^{\frac{1}{p}-\frac{1}{q}}\, \tilde{\mu}_j(A)\right\|_q.$$

As a particular case, when $q = \infty$, these are often called the weak Schatten spaces $\mathfrak{S}^{p,\infty} = \{A \in \mathcal{K},\ \sup_{j\geq 0}(j^{\frac{1}{p}}\, \mu_j(A)) < \infty\}$. They satisfy for any $p \in [1,\infty)$, [Sim05, p.18]

$$\frac{1}{p'}\,\|A\|_{p,\infty} \leq \sup_{j\geq 0}\left(j^{1/p}\mu_j(A)\right) \leq \|A\|_{p,\infty}.$$

It is sometimes also conventient to define $\mathring{\mathfrak{S}}^{p,\infty} = \{A \in \mathfrak{S}^{p,\infty},\ j^{\frac{1}{p}}\, \mu_j(A) \underset{j\to\infty}{\to} 0\}$.

Duals. As for functions, one can identify linear forms acting on compact operators to operators through the duality product $(A|B) = \mathrm{Tr}(A^*B)$. Birman and Solomyak [BS77, Equation (1.15)] give the following results concerning the duals of the above defined spaces. For any $(p,q) \in (1,\infty)\times[1,\infty)$,

$$(\mathfrak{S}^\infty)' = \mathfrak{S}^1, \qquad (\mathfrak{S}^{p,q})' = \mathfrak{S}^{p',q'}, \qquad (\mathring{\mathfrak{S}}^{p,\infty})' = \mathfrak{S}^{p',1}.$$

Embedding. Again, similarly as for Lorentz spaces, for any fixed p, these spaces are ordered depending on the second parameter q, but the first index p is the most important, and the spaces follow the same inclusions as sequence spaces and Schatten spaces. This yields (see [BS77, Equations (1.2), (1.3), (1.4)])

$$\begin{aligned} \mathfrak{S}^{p_0,q_0} &\subset \mathfrak{S}^{p_1,q_1} && \text{if } p_0 < p_1 \\ \mathfrak{S}^{p,q_0} &\subset \mathfrak{S}^{p,q_1} && \text{if } q_0 < q_1, (p,q_0,q_1) \in (0,\infty]^3 \\ \mathfrak{S}^{p,q} &\subset \mathring{\mathfrak{S}}^{p,\infty} && \text{if } (p,q) \in (0,\infty)^2. \end{aligned}$$

Interpolation. One can look at the real and complex interpolation of Schatten and weak Schatten spaces. Let $(p_0,p_1) \in [1,\infty]^2$ and for $\theta \in (0,1)$ define the intermediate exponent p_θ by $\frac{1}{p_\theta} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}$. Without surprises, real interpolation of Schatten spaces gives $\mathfrak{S}^{p,q}$ spaces (see e.g. [Tri78, 1.19.7])

$$\begin{aligned} (\mathfrak{S}^1, \mathfrak{S}^\infty)_{\theta,q} &= \mathfrak{S}^{p_\theta,q} && \text{if } q \in (1,\infty), p_0 = 1, p_1 = \infty \\ (\mathfrak{S}^{p_0}, \mathfrak{S}^{p_1})_{\theta,p_\theta} &= \mathfrak{S}^{p_\theta}. \end{aligned}$$

while complex interpolation of Schatten spaces give other Schatten spaces

$$[\mathfrak{S}^1, \mathfrak{S}^\infty]_\theta = \mathfrak{S}^{p_\theta}.$$

5.5 Inequalities for singular values and Schatten norms

5.5.1 Tensor products

In a general Hilbert space $\mathcal{H}$, one can define the tensor product of n elements by

$$(\psi_1 \otimes \cdots \otimes \psi_n) : (\varphi_1, \ldots, \varphi_n) \mapsto \prod_{k=1}^{n} \langle \psi_k \,|\, \varphi_k \rangle \,.$$

Remark 5.5.1. In the case when $\mathcal{H} = L^2$, this is equivalent (by Riesz theorem) to define

$$(\psi_1 \otimes \cdots \otimes \psi_n)(x_1, \ldots, x_n) = \psi_1(x_1) \ldots \psi_n(x_n) \,.$$

The completion of the span of the vectors of this form is denoted $\mathcal{H}^{\otimes n}$, and any Hilbert basis $(\phi_j)_{j\in J}$ of $\mathcal{H}$ defines an Hilbert basis $(\phi_1 \otimes \cdots \otimes \phi_n)$ of $\mathcal{H}^{\otimes n}$. Similarly, one associates to any operators $(A_1, \ldots, A_n) \in \mathcal{L}(\mathcal{H})^n$ the tensor product $A_1 \otimes \cdots \otimes A_n \in \mathcal{L}(\mathcal{H}^{\otimes n})$ defined by

$$(A_1 \otimes \cdots \otimes A_n)(\psi_1 \otimes \cdots \otimes \psi_n) = (A_1\psi_1 \otimes \cdots \otimes A_n\psi_n) \,,$$

and extended to $\mathcal{H}^{\otimes n}$ by linearity. If the A_j are all bounded operators, this defines a bounded operator with norm

$$\|A_1 \otimes \cdots \otimes A_n\|_\infty = \|A_1\|_\infty \ldots \|A_n\|_\infty \,.$$

In particular, in the case of an operator $A \in \mathcal{L}(\mathcal{H})$, one can associate an operator $\Gamma_n(A) \in \mathcal{L}(\mathcal{H}^{\otimes n})$ defined by

$$\Gamma_n(A) = A^{\otimes n} = A \otimes \cdots \otimes A \,.$$

Notice that $\Gamma_n(AB) = \Gamma_n(A)\,\Gamma_n(B)$.

Antisymmetric tensor products. We can also define the antisymmetric tensor product for $\psi_1 \otimes \cdots \otimes \psi_n \in \mathcal{H}^{\otimes n}$ by

$$\psi_1 \wedge \cdots \wedge \psi_n := \frac{1}{\sqrt{n!}} \sum_\sigma (-1)^\sigma \, \psi_{\sigma(1)} \otimes \cdots \otimes \psi_{\sigma(n)} \,,$$

where the sum goes over all permutations σ of $\{ 1, \ldots, n \}$ and $(-1)^\sigma$ is the sign of the permutation.

Remark 5.5.2. When $\mathcal{H} = L^2$, then the antisymmetric tensor product gives the function $\psi_1 \wedge \cdots \wedge \psi_n(x_1, \ldots, x_n) = (n!)^{-1/2} \det(\psi_j(x_k))_{1\leq j,k\leq n}$ called a Slater determinant.

The space of antisymmetric tensors, denoted by $\mathcal{H}^{\wedge n}$, is then the completion of the span of the vectors of this form. If $n = 0$, we define $\mathcal{H}^{\wedge 0} := \mathbb{C}$. Elementary computations show that the factor $1/\sqrt{n!}$ is taken such that if in particular $(\phi_j)_{j\in J}$ is an orthonormal basis of $\mathcal{H}$, then $(\phi_{k_1} \wedge \cdots \wedge \phi_{k_n})_{k_1 < \cdots < k_n \in J}$ is an orthonormal basis for $\mathcal{H}^{\wedge n}$. On can also prove that the orthogonal projection on $\mathcal{H}^{\wedge n}$ is the extension by linearity of the operator defined for $\psi_1 \otimes \cdots \otimes \psi_n \in \mathcal{H}^{\otimes n}$ by

$$P_\wedge \left(\psi_1 \otimes \cdots \otimes \psi_n\right) := \frac{1}{\sqrt{n!}}\, \psi_1 \wedge \cdots \wedge \psi_n = \frac{1}{n!} \sum_\sigma (-1)^\sigma \, \psi_{\sigma(1)} \otimes \cdots \otimes \psi_{\sigma(n)} \,.$$

For an operator $A \in \mathcal{L}(\mathcal{H})$, we can associate the operator

$$\Lambda_n(A) := \Gamma_n(A)\, P_\wedge = P_\wedge\, \Gamma_n(A)\,,$$

which restricted to $\mathcal{H}^{\wedge n}$ is nothing but the restriction of the operator $\Gamma_n(A)$ to $\mathcal{H}^{\wedge n}$. In particular, it satisfies

$$\Lambda_n(AB) = \Lambda_n(A)\,\Lambda_n(B)\,. \tag{50}$$

If A is a bounded operator, then $\Lambda_n(A)$ is also a bounded operator and if A is compact, one obtains the following (see e.g. [Sim05, (1.14)]).

Proposition 5.9. *Let $A \in \mathcal{K}$ and $n \in \mathbb{N}$. Then $\Lambda_n(A) \in \mathcal{L}^\infty(\mathcal{H}^{\wedge n})$ and*

$$\|\Lambda_n(A)\|_{\mathcal{L}^\infty(\mathcal{H}^{\wedge n})} = \prod_{j=0}^{n-1} \mu_j(A)\,. \tag{51}$$

Proof. if A is a positive compact self-adjoint operator and $\psi_0, \ldots, \psi_n, \ldots$ is a complete set of orthogonal eigenvectors for A, then $(\psi_{j_1}, \ldots, \psi_{j_n})_{0 \le j_1 < \cdots < j_n}$ is a complete set of eigenvectors for $\Lambda_n(A)$, which leads to Equation (51) by taking the first eigenvalue. The general case follows from the fact that $|\Lambda_n(A)| = \Lambda_n(|A|)$. □

5.5.2 Horn's Theorems and Hölder's inequality

From the previous proposition we deduce the following theorem.

Theorem 5.10 (Horn [Hor50])**.** *For any $(A, B) \in \mathcal{K}^2$ and $n \in \mathbb{N}$,*

$$\prod_{j=0}^{n} \mu_j(AB) \le \prod_{j=0}^{n} \mu_j(A)\, \mu_j(B)\,.$$

Proof. It follows from Formula (50), that

$$\|\Lambda_n(AB)\|_{\mathcal{L}^\infty(\mathcal{H}^{\wedge n})} \le \|\Lambda_n(A)\|_{\mathcal{L}^\infty(\mathcal{H}^{\wedge n})}\, \|\Lambda_n(B)\|_{\mathcal{L}^\infty(\mathcal{H}^{\wedge n})}\,,$$

hence the result follows by Equation (51). □

This theorem allows to deduce a lot of inequalities on singular values. To obtain them, we first introduce the **decreasing rearrangement** of a sequence. If $a = (a_k)_{k \ge 0}$ is a sequence of complex numbers, then we denote by $a^* := (a_k^*)_{k \ge 0}$ the decreasing sequence such that for all $c \ge 0$, $\{\, k \ge 0, a_k^* = c \,\}$ and $\{\, k \ge 0, |a_k| = c \,\}$ have the same number of elements. The following rearrangement inequalities hold.

Lemma 5.11.

$$\sum_{k \ge 0} |a_k\, b_k| \le \sum_{k \ge 0} a_k^*\, b_k^*\,.$$

Proof. Suppose first that the sums have a finite number of terms, i.e. they are sums over k such that $0 \le k \le n$ for some $n \in \mathbb{N}$. Then we can renumber the a_k and b_k in such a way that $|a_k|$ is decreasing without changing the value of the sum. Then we can write

$$\sum_{k=0}^{n} |a_k\, b_k| = |a_n| \sum_{k=0}^{n} |b_k| + (|a_{n-1}| - |a_n|) \sum_{k=0}^{n-1} |b_k| + \cdots + (|a_0| - |a_1|)\, |b_0|$$

and since for any $1 \le m \le n$,

$$\sum_{k=0}^{m} |b_k| \le \sum_{k=0}^{m} b_k^*$$

we deduce the result for the case of a finite number of terms. The case of an infinite number of terms follows from a limiting argument letting $n \to \infty$. □

Lemma 5.12. *Assume $a, b \in \mathbb{C}^n$ are such that*

$$\forall m \in \{1, \dots, n\}, \qquad \sum_{k=0}^{m} b_k^* \le \sum_{k=0}^{m} a_k^* .$$

Then for any function $\Phi : \mathbb{R}_+^n \to \mathbb{R}$ so that $\Phi_* : c \mapsto \Phi(c^*)$ is convex on $\mathbb{C}^n$

$$\Phi_*(b) \le \Phi_*(a) .$$

Proof. The proof consists in showing that $(b_1, \dots, b_n)$ is in the convex hull of the points $c \in \mathbb{C}^n$ such that $c^* = a$, i.e.

$$b = \sum_{k=1}^{N} \theta_k \, c^{(k)}$$

which is proved using the previous lemma. (See [Sim05, Theorem 1.9]) □

Lemma 5.13. *Assume $(a, b) \in \mathbb{C}^{2n}$ are positive decreasing sequences such that*

$$\forall m \in \{1, \dots, n\}, \qquad \prod_{k=1}^{m} b_k \le \prod_{k=1}^{m} a_k . \tag{52}$$

Then for any increasing function $\Psi \in C^0(\mathbb{R}_+)$ with $t \mapsto \Psi(e^t)$ convex,

$$\sum_{k=1}^{n} \Psi(b_k) \le \sum_{k=1}^{n} \Psi(a_k) .$$

Proof. Replacing a_k by a_k/θ, b_k by b_k/θ and $\Psi(x)$ by $\Psi(\theta x)$, we can suppose that the a_k and b_k are larger than 1. Therefore, taking the logarithm of (52), we obtain

$$\sum_{k=1}^{m} \ln(b_k) \le \sum_{k=1}^{m} \ln(a_k) .$$

and we conclude by previous lemma with $\Phi(x) = \sum_k \Psi(e^x)$. □

Theorem 5.14 (Horn [Hor50])**.** *Let $\Psi : \mathbb{R}_+ \to \mathbb{R}_+$ be an increasing function so that $\Psi(e^t)$ is convex. Then for any $(A, B) \in \mathcal{K}^2$*

$$\sum_{j \ge 0} \Psi(\mu_j(AB)) \le \sum_{j \ge 0} \Psi(\mu_j(A)\, \mu_j(B)) . \tag{53}$$

and so in particular, with $\Psi = |\cdot|^p$, one deduces Hölder's inequality (see [Sim05, Theorem 2.8])

$$\|AB\|_p \le \|A\|_q \, \|B\|_r$$

for any $(p, q, r) \in [1, \infty]^3$ such that

$$\frac{1}{p} = \frac{1}{q} + \frac{1}{r} .$$

Remark 5.5.3. There is also a version of Hölder's inequality using weak Schatten spaces analogous to the weak Lebesgue spaces, useful to handle singular operators (see e.g. [Sim05, Theorem 2.8])

$$\|AB\|_{p,\infty} \leq p' \|A\|_{q,\infty} \|B\|_{r,\infty} .$$

Remark 5.5.4. Another inequality similar to Horn's theorem is the following Weyl inequality. Let $A \in \mathcal{K}$ and $n \in \mathbb{N}$, then

$$\prod_{j=0}^{n} |\lambda_j(A)| \leq \prod_{j=0}^{n} \mu_j(A) .$$

We deduce similarly from it that

$$\sum_{j\geq 0} \Psi(|\lambda_j(A)|) \leq \sum_{j\geq 0} \Psi(\mu_j(A)) . \tag{54}$$

5.5.3 Triangle inequality for Schatten norms

The Schatten norms are of course norms, i.e. one can prove that they satisfy the triangle inequality.

Proposition 5.15. *Let $p \in [1, \infty]$ and $A, B \in \mathcal{L}^\infty(H)$. Then*

$$\|A + B\|_p \leq \|A\|_p + \|B\|_p .$$

Another "reversed" inequality also holds for positive operators, whenever $p < \infty$ and $(A, B) \in (\mathfrak{S}^p_+)^2$, then (see [Sim05, Theorem 1.22])

$$\|A\|_p^p + \|B\|_p^p \leq \|A + B\|_p^p .$$

5.5.4 Araki–Lieb–Thirring–Heinz inequalities

Even if the trace is invariant by cyclic permutations of operators and the Schatten norms are invariant by taking the adjoint, the non-commutativity is still important in the other cases. This is a pure quantum feature. One can however obtain inequalities between the norms of products of operators depending on the order.

Theorem 5.16 (Heinz inequality [Hei51])**.** *Let A and B be positive bounded linear operators. Then for any $\theta \in [0, 1]$,*

$$\left\|A^\theta B^\theta\right\|_\infty \leq \|AB\|_\infty^\theta .$$

Equivalently, for any $p \geq 1$,

$$\|AB\|_\infty^p \leq \|A^p B^p\|_\infty . \tag{55}$$

The proof we give is inspired by [Fur89].

Proof. Let $S = \{\, \theta \in [0, 1], \left\|A^\theta B^\theta\right\|_\infty \leq \|AB\|_\infty^\theta \,\}$. Since S is a closed set containing 0 and 1, we just have to prove that $(\theta_1, \theta_2) \in S^2 \implies \theta = (\theta_1 + \theta_2)/2 \in S$. But now, since the spectral radius verifies $r(AB) = r(BA)$ and $B^\theta A^{2\theta} B^\theta \geq 0$,

$$\begin{aligned}\left\|A^\theta B^\theta\right\|_\infty^2 &= \left\|B^\theta A^{2\theta} B^\theta\right\|_\infty = r(B^\theta A^{2\theta} B^\theta) = r(B^{\theta_1} A^{\theta_1+\theta_2} B^{\theta_2}) \\ &\leq \left\|B^{\theta_1} A^{\theta_1+\theta_2} B^{\theta_2}\right\|_\infty \leq \left\|B^{\theta_1} A^{\theta_1}\right\|_\infty \left\|A^{\theta_2} B^{\theta_2}\right\|_\infty\end{aligned}$$

and now since $(\theta_1, \theta_2) \in S^2$, it leads to

$$\left\|A^\theta B^\theta\right\|_\infty^2 \leq \|BA\|_\infty^{\theta_1} \|BA\|_\infty^{\theta_2} = \|BA\|_\infty^{2\theta}$$

and so $\theta \in S$. □

More generally, the Araki–Lieb–Thirring inequality [Ara90] states what happens for Schatten norms, with possibly unbounded operators.

Theorem 5.17 (Araki–Lieb–Thirring). *Let A and B be positive self-adjoint operators and $(p, r) \in [1, \infty) \times \mathbb{R}_+$*

$$\|AB\|_{pr}^p \leq \|A^p B^p\|_r \text{ for any } p \geq 1. \tag{56}$$

Equivalently, since $|AB| = (BA^2B)^{\frac{1}{2}}$, we can rewrite Inequality (56) as

$$\operatorname{Tr}((BAB)^{pr}) \leq \operatorname{Tr}((B^p A^p B^p)^r)\,. \tag{57}$$

Remark 5.5.5. A particularly simple case, useful to remember the general inequality, is the case $r = 1$ and $p = 2$. In this case, one simply writes

$$\|AB\|_2^2 = \operatorname{Tr}\big(BA^2B\big) = \operatorname{Tr}\big(A^2B^2\big) \leq \left\|A^2B^2\right\|_1.$$

Remark 5.5.6. As noticed in [Sim05, Theorem 8.1], the same strategy of proof as these two theorems shows that if $(A, B) \in (\mathcal{L}^\infty)^2$ are such that AB is self-adjoint, then for any $p \in [1, \infty)$,

$$\|AB\|_p \leq \|BA\|_p\,.$$

Proof of Theorem 5.17. Assume that A and B are positive matrices and let $C_q = A^q B^q$. Then by Inequality (51), for $q = 1$ or $q = p$ it holds

$$\left\|\Lambda_n(|C_q|^2)\right\|_\infty = \prod_{j=0}^{n-1} \mu_j(|C_q|^2)\,.$$

But for the operator norm it holds

$$\left\|\Lambda_n(|C_q|^2)\right\|_\infty = \left\|\Lambda_n(C_q)^*\Lambda_n(C_q)\right\|_\infty = \left\|\Lambda_n(C_q)\right\|_\infty^2 = \left\|\Lambda_n(A)^q\Lambda_n(B)^q\right\|_\infty^2.$$

Therefore, by the Heinz inequality (55)

$$\left\|\Lambda_n(|C_1|^2)\right\|_\infty^p = \left\|\Lambda_n(A)\,\Lambda_n(B)\right\|_\infty^{2p} \leq \left\|\Lambda_n(A)^p\Lambda_n(B)^p\right\|_\infty^2 = \left\|\Lambda_n(|C_p|^2)\right\|_\infty$$

and so

$$\prod_{j=0}^{n-1} \mu_j\big(\,|AB|^{2p}\,\big) = \prod_{j=0}^{n-1} \mu_j\big(\,|AB|^2\,\big)^p \leq \prod_{j=0}^{n-1} \mu_j\big(\,|A^pB^p|^2\,\big).$$

which proves the result by Lemma 5.13 with $\Psi(x) = x^{r/2}$. The general case follows by approximation arguments detailed in [Ara90]. □

5.6 Factorized operators $f(x)\, g(-i\nabla)$

5.6.1 The Kato–Seiler–Simon inequality

A special case of operators are operators of the form $f(x)\, g(-i\nabla)$. For these operators, the Kato–Seiler–Simon inequality and Cwikel inequality (see [Sim05, Theorem 4.1 and Theorem 4.2] and [Cwi77]) state that

$$\|f(x)\, g(-i\nabla)\|_p \leq \frac{1}{(2\pi)^{d/p}} \|f\|_{L^p} \|g\|_{L^p} \qquad \text{when } p \in [2,\infty]$$
$$\|f(x)\, g(-i\nabla)\|_{p,\infty} \leq C_{d,p} \|f\|_{L^p} \|g\|_{L^{p,\infty}} \qquad \text{when } p \in (2,\infty)$$

where $C_{d,p}$ is a constant depending on d and p. These inequalities are very intuitive from a semiclassical point of view. Replacing g by $g(h\cdot)$, they can indeed be written with $\boldsymbol{p} = -i\hbar\nabla$ and the semiclassical Schatten norms defined in Equation (41) (i.e. $\|\boldsymbol{\rho}\|_{\mathcal{L}^p} = h^{d/p} \|\boldsymbol{\rho}\|_p$) under the following form.

Proposition 5.18. *For any $p \in [2,\infty]$ and any measurable functions $f, g : \mathbb{R}^d \to \mathbb{C}$*

$$\|f(x)\, g(\boldsymbol{p})\|_p \leq \|f\|_{L^p} \|g\|_{L^p} \tag{58}$$

with equality in the case $p = 2$, and if $p \in (2,\infty)$,

$$\|f(x)\, g(\boldsymbol{p})\|_{p,\infty} \leq \|f\|_{L^p} \|g\|_{L^{p,\infty}}$$

where the norms $\mathcal{L}^{p,\infty}$ are defined with the same scaling as the norms $\mathcal{L}^p$.

In particular, noticing that $\|f\|_{L^p} \|g\|_{L^p} = \|f(x)\, g(\xi)\|_{L^p(\mathbb{R}^{2d})}$, this can be seen as a comparison between the quantum and classical norms of functions that are factorized in phase space.

Proof of Inequality (58). Noticing that $\boldsymbol{\rho} = B(f,g) := f(x)\, g(\boldsymbol{p})$ is bilinear, the proof for a general p will follow by (bilinear) complex interpolation if we can prove the endpoints cases $p = 2$ and $p = \infty$. In the case $p = \infty$, it follows by Plancherel theorem that

$$\begin{aligned} \|f(x) g(\boldsymbol{p})\psi\|_{L^2} &\leq \|f\|_{L^\infty} \|g(\boldsymbol{p})\psi\|_{L^2} = \|f\|_{L^\infty} \left\| g(h\, y)\, \widehat{\psi}(y) \right\|_{L^2} \\ &\leq \|f\|_{L^\infty} \|g\|_{L^\infty} \|\psi\|_{L^2} \end{aligned}$$

which gives the result in this case. In the case $p = 2$, we can use the fact that the Hilbert–Schmidt norm is just given as the L^2 norm of the integral kernel of the operator. Since

$$\boldsymbol{\rho}(x,y) = \frac{1}{h^d} f(x)\, \widehat{g}(\tfrac{y-x}{h}),$$

it yields

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^2}^2 = h^d \operatorname{Tr}\Big(|\boldsymbol{\rho}|^2\Big) = \frac{1}{h^d} \int_{\mathbb{R}^d} \left| f(x)\, \widehat{g}(\tfrac{y-x}{h}) \right|^2 = \|f\|_{L^2}^2 \|g\|_{L^2}^2,$$

which shows that in the case $p = 2$, one even more gets an identity. □

Remark 5.6.1. Related inequalities in weighted spaces are proved by Birman–Solomyak [BS77]. Using the fact that $\mu_j(g_1\, A\, g_0) = \mu_j(A_{L^2(g_0)\to L^2(g_1)})$, their results imply the following inequalities. Let $s_0 = s_1 + s_2 \geq 0$, $(p_0, p_1, p_2, q_1, q_2) \in (\frac{2}{3}, 2] \times [2,\infty)^2 \times (2,\infty)^2$ satisfying

$$\forall \mathrm{i} \in \{0,1,2\},\ \frac{1}{p_{\mathrm{i}}} + \frac{1}{q_{\mathrm{i}}} = \frac{1}{2} + \frac{s_{\mathrm{i}}}{d} \quad \text{(with } q_0 = \infty\text{)}.$$

Then there exists a constant $C > 0$ such that for any $(f,g) \in L^{q_1}(\mathbb{R}^d) \times L^{q_2}(\mathbb{R}^d)$ and integral operator A with kernel $K_A \in W_x^{s_1,p_1} W_y^{s_2,p_2}$,

$$\|f\, A\, g\|_{p_0,\infty} \leq C\, \|K_A\|_{W_x^{s_1,p_1} W_y^{s_2,p_2}}\, \|f\|_{L^{q_1}}\, \|g\|_{L^{q_2}}\,.$$

In particular, if $\frac{1}{p_1} + \frac{1}{q_1} = \frac{1}{2}$ and $\frac{1}{p_2} + \frac{1}{q_2} = \frac{1}{2}$, then

$$\|f\, A\, g\|_{2,\infty} \leq C\, \|K_A\|_{L_x^{p_1} L_y^{p_2}}\, \|f\|_{L^{q_1}}\, \|g\|_{L^{q_2}}\,.$$

5.6.2 The Birman–Solomyak inequality

One can notice that the Kato–Seiler–Simon inequality unfortunately only works when $p \geq 2$. When $p \in [1,2)$, one has to replace the L^p norms of the functions by a locally stronger norm. We denote by $Q_\varepsilon(x) = x + [-\varepsilon/2, \varepsilon/2]^d \subset B_{\varepsilon\sqrt{d}/2}(x)$ the cubes of center x and length ε. Then the Birman–Solomyak norms are defined by

$$\|u\|_{\mathfrak{L}^{p,q}} = \left(\sum_{n\in\mathbb{Z}^d} \left(\int_{Q_1(n)} |u|^q\right)^{p/q}\right)^{1/p} =: \|u\|_{\ell^p(L^q(Q_1(n)))}\,.$$

Equivalent norms are given by $\|u(x+z)\|_{L_x^p L_z^q(Q_1(0))}$. The Birman–Solomyak inequality (see [Sim05, Theorem 4.5]) states that for any $p \in [1,2]$, there exists a constant $C > 0$ such that

$$\|f(x)\, g(-i\nabla)\|_p \leq C\, \|f\|_{\mathfrak{L}^{p,2}}\, \|g\|_{\mathfrak{L}^{p,2}}\,. \tag{59}$$

As noticed by Simon [Sim05, Theorem 4.7], these norms are optimal at least in the case $p = 1$ in the sense that

$$f(x)\, g(-i\nabla) \in \mathfrak{S}^1 \iff (f,g) \in (\mathfrak{L}_1^{1,2})^2.$$

To keep track of the semiclassical behavior, we can define norms depending on a small parameter $\varepsilon > 0$

$$\|u\|_{\mathfrak{L}_\varepsilon^{p,q}} := \left(\varepsilon^d \sum_{x\in\varepsilon\mathbb{Z}^d} \left(\frac{1}{\varepsilon^d}\int_{Q_\varepsilon(x)} |u|^q\right)^{p/q}\right)^{1/p} = \varepsilon^{d/p}\, \|u(\varepsilon\,\cdot)\|_{\mathfrak{L}_1^{p,q}}$$

which generalize the previously defined distance in the sense that $\mathfrak{L}^{p,q} = \mathfrak{L}_1^{p,q}$. Since $f(x)\, g(\boldsymbol{p}) = \mathsf{h}_a^*\, f(ax)\, g(\frac{\boldsymbol{p}}{a})\, \mathsf{h}_a$ with h_a the unitary dilatation operators, taking $a = \sqrt{h}$ gives $f(x)\, g(\boldsymbol{p}) = \mathsf{h}_a^*\, f(\sqrt{h}\, x)\, g(\sqrt{h}\frac{\nabla}{2\pi})\, \mathsf{h}_a$ and so the Birman–Solomyak inequality (59) can be written in the following way.

Corollary 5.19 (Semiclassical Birman–Solomyak inequality)**.** *Let $p \in [1,2]$. Then there exists $C_{d,p} > 0$ such that for any $f, g : \mathbb{R}^d \to \mathbb{R}^d$,*

$$\|f(x)\, g(\boldsymbol{p})\|_{\mathcal{L}^p} \leq C_{d,p}\, \|f\|_{\mathfrak{L}_{\sqrt{h}}^{p,2}}\, \|g\|_{\mathfrak{L}_{\sqrt{h}}^{p,2}}\,.$$

Notice that $\|u\|_{\mathfrak{L}^{p,p}_\varepsilon} = \|u\|_{L^p}$ and if $q_1 \leq q_2$, then $\|u\|_{\mathfrak{L}^{p,q_1}_\varepsilon} \leq \|u\|_{\mathfrak{L}^{p,q_2}_\varepsilon}$. Therefore, if $p \leq q$,

$$\|u\|_{\mathfrak{L}^{p,1}_\varepsilon} \leq \|u\|_{L^p} \leq \|u\|_{\mathfrak{L}^{p,q}_\varepsilon} \leq \|u\|_{\mathfrak{L}^{p,\infty}_\varepsilon}$$

so that the $\mathfrak{L}^{p,2}_{\sqrt{h}}$ norms are indeed larger than the L^p norms when $p < 2$. At fixed ε, they even more control the L^2 norms and more generally for $q \geq p$ one has

$$\varepsilon^{d\left(\frac{1}{p}-\frac{1}{q}\right)} \|u\|_{L^q} \leq \|u\|_{\mathfrak{L}^{p,q}_\varepsilon} .$$

However, the above inequality is trivial in the limit $\varepsilon \to 0$, and the $\mathfrak{L}^{p,q}_\varepsilon$ norms converge as expected to L^p norms. One can get a quantitative statement.

Proposition 5.20. *Let $p \leq q$ and $\varepsilon \in (0,1)$. Then there exists $C_d > 0$ such that for any $u : \mathbb{R}^d \to \mathbb{R}^d$,*

$$\|u\|_{L^p} \leq \|u\|_{\mathfrak{L}^{p,q}_\varepsilon} \leq \|u\|_{L^p} + C_d\, \varepsilon \,\|\nabla u\|_{\mathfrak{L}^{p,q}} \tag{60}$$

Remark 5.6.2. It is not difficult to see that by Hölder's inequality, $\|u\|_{\mathfrak{L}^{p,q}_\varepsilon} \leq C\, \|u\|_{L^q(m)}$ where $m(x) = \langle x\rangle^k$ with $k > d\left(\frac{1}{p}-\frac{1}{q}\right)$. Therefore for any $p \in [1,2]$,

$$\|f(x)\, g(\boldsymbol{p})\|_{\mathcal{L}^p} \leq C_p \left(\|f\|_{L^p} + \sqrt{h}\,\|\nabla f\|_{L^2(m)}\right)\left(\|g\|_{L^p} + \sqrt{h}\,\|\nabla g\|_{L^2(m)}\right)$$

Proof of Inequality (60). By the triangle inequality and the fact that $\mathfrak{L}^{p,p}_\varepsilon = L^p$,

$$\begin{aligned}\left|\|u\|_{\mathfrak{L}^{p,q}_\varepsilon} - \|u\|_{L^p}\right| &= \varepsilon^{d/p}\left|\|u(\varepsilon\,\cdot)\|_{\ell^p(L^q(Q_1(n)))} - \|u(\varepsilon\,\cdot)\|_{\ell^p(L^p(Q_1(n)))}\right| \\ &\leq \varepsilon^{d/p}\left\|\|u(\varepsilon\,\cdot)\|_{L^q(Q_1(n))} - \|u(\varepsilon\,\cdot)\|_{L^p(Q_1(n))}\right\|_{\ell^p}\end{aligned}$$

Since the cubes $Q_1(n)$ are of volume 1, $\|1\|_{L^p(Q_1(n))} = \|1\|_{L^q(Q_1(n))} = 1$, and so it yields

$$\begin{aligned}\left|\|u\|_{\mathfrak{L}^{p,q}_\varepsilon} - \|u\|_{L^p}\right| &\leq \varepsilon^{d/p}\left\|\|u(\varepsilon\, y)\|_{L^p_x(Q_1(n))L^q_y(Q_1(n))} - \|u(\varepsilon\, x)\|_{L^p_x(Q_1(n))L^q_y(Q_1(n))}\right\|_{\ell^p} \\ &\leq \varepsilon^{d/p}\left\|\|u(\varepsilon\, x) - u(\varepsilon\, y)\|_{L^p_x(Q_1(n))L^q_y(Q_1(n))}\right\|_{\ell^p}\end{aligned}$$

Since $u(\varepsilon\, x) - u(\varepsilon\,(x+z)) = \varepsilon\left|z\cdot\int_0^1 \nabla u(x+\theta\,\varepsilon z)\,\mathrm{d}\theta\right|$ by the fundamental theorem of calculus, it finally leads to

$$\begin{aligned}\left|\|u\|_{\mathfrak{L}^{p,q}_\varepsilon} - \|u\|_{L^p}\right| &\leq \varepsilon^{d/p}\left\|\|u(\varepsilon\, x) - u(\varepsilon\,(x+z))\|_{L^p_x(Q_1(n))L^q_z(Q_2(0))}\right\|_{\ell^p} \\ &\leq \sqrt{d}\,\varepsilon\int_0^1 \|\nabla u(x+\theta\,\varepsilon z)\|_{L^p_x L^q_z(Q_2(0))}\,\mathrm{d}\theta.\end{aligned}$$

To conclude use the fact that $\|u(x+\theta z)\|_{L^p_x L^q_z(Q_c(0))} \leq \lceil 1+\theta c\rceil^d\,\|u\|_{\mathfrak{L}^{p,q}}$ to get the result with $C_d = \sup_{\varepsilon>0}\int_0^1 \lceil 1+2\theta\varepsilon\rceil^d\,\mathrm{d}\theta$. □

5.7 Schrödinger eigenvalues and interpolation inequalities

5.7.1 The Kinetic interpolation inequality

The Lieb–Thirring inequality [LT76] can be thought of as the quantum analogue of the kinetic interpolation inequality presented in Proposition 4.1, and more precisely the case $k = 0$ which we recall in the following proposition.

Proposition 5.21. *Let $n \geq 0$ and $r \in [1,\infty]$. Then for any non-negative function $f \in L^1(\mathbb{R}^{2d})$*

$$\|\rho_f\|_{L^p} \leq \mathcal{C}^{\mathrm{cl}}_{d,n,r} \, \|f\|^{\theta}_{L^r(\mathbb{R}^{2d})} \left(\iint_{\mathbb{R}^{2d}} f\,|\xi|^n \,\mathrm{d}x\,\mathrm{d}\xi\right)^{1-\theta} \tag{61}$$

with $\rho_f = \int_{\mathbb{R}^d} f\,\mathrm{d}\xi$, $p' = r' + \frac{d}{n}$ and $\theta = \frac{r'}{p'}$.

Remark 5.7.1. The optimal constant is given in Equation (**??**) in the next section. When $r = \infty$, then $p' = 1 + \frac{d}{n}$ so $p = 1 + \frac{n}{d}$ and $\theta = 1/p'$, $1-\theta = 1/p$. In particular the optimal constant is given by

$$\mathcal{C}^{\mathrm{cl}}_{d,n} = p^{\frac{1}{p}} \left(\frac{\omega_d}{d}\right)^{\frac{1}{p'}}$$

and a minimizer is given by $f(x,\xi) = \mathbb{1}_{\omega_d |\xi|^d \leq d\,\rho_f(x)}$, this is the *bathtub filling principle*.

Theorem 5.22 (Semiclassical kinetic interpolation inequality)**.** *It holds*

$$\|\rho_{\boldsymbol{\rho}}\|_{L^p} \leq \mathcal{C}_{d,n,r} \left(h^d \operatorname{Tr}(|\boldsymbol{p}|^n \boldsymbol{\rho})\right)^{1-\theta} \|\boldsymbol{\rho}\|^{\theta}_{\mathcal{L}^r}\,, \tag{62}$$

with $p' = r' + d/n$, $\theta = \frac{r'}{p'}$ and $\theta^\theta\,(1-\theta)^{1-\theta}\,\mathcal{C}_{d,n,r} = \mathcal{L}^{1/p'}_{r',d,n}$.

Remark 5.7.2. When $r = \infty$, we write $\mathcal{C}_{d,n} := \mathcal{C}_{d,n,\infty}$ and then

$$\|\rho_{\boldsymbol{\rho}}\|_{L^p} \leq \mathcal{C}_{d,n} \left(h^d \operatorname{Tr}(|\boldsymbol{p}|^n \boldsymbol{\rho})\right)^{1/p} \|\boldsymbol{\rho}\|^{1/p'}_{\mathcal{L}^\infty}\,,$$

which for $n = 2$ and $d = 3$ reads

$$\|\rho_{\boldsymbol{\rho}}\|_{L^{5/3}} \leq \mathcal{C}_{3,2} \left(h^3 \operatorname{Tr}\Big(|\boldsymbol{p}|^2 \boldsymbol{\rho}\Big)\right)^{3/5} \|\boldsymbol{\rho}\|^{2/5}_{\mathcal{L}^\infty}\,,$$

In the original work of Lieb and Thirring [LT76], fermions are considered and so $\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} \leq 1$, and the inequality can be written

$$h^3 \operatorname{Tr}\Big(|\boldsymbol{p}|^2 \boldsymbol{\rho}\Big) \geq \mathcal{K}_{3,2} \int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}^{5/3},$$

where $\mathcal{K}_{d,n} = \mathcal{C}^{-p}_{d,n}$.

We can follow the proof of the analogous inequality in the non-quantum case to obtain a simple proof, which however does not give the optimal constant.

Proof in the case $r = \infty$. We define the operators $\boldsymbol{\chi}_\lambda := \mathbb{1}_{|\boldsymbol{p}|^n \leq \lambda}$ and $\boldsymbol{\chi}^{\mathrm{c}}_\lambda := \mathbb{1}_{|\boldsymbol{p}|^n > \lambda}$. Then notice that $\|\boldsymbol{\rho}\|_{\mathcal{L}^2_\xi}$, which is the function of x defined by

$$\|\boldsymbol{\rho}\|^2_{\mathcal{L}^2_\xi} := \rho_{|\boldsymbol{\rho}|^2}(x) = h^d\,|\boldsymbol{\rho}|^2\,(x,x) = h^d \int_{\mathbb{R}^d} |\boldsymbol{\rho}(x,y)|^2 \,\mathrm{d}y$$

is a norm for any fixed $x \in \mathbb{R}^d$, which satisfies $\|\boldsymbol{\rho}\|_{L^2_x(\mathcal{L}^2_\xi)} := \|\|\boldsymbol{\rho}\|_{\mathcal{L}^2_\xi}\|_{L^2_x} = \|\boldsymbol{\rho}\|_{\mathcal{L}^2}$. Hence by the triangle inequality it holds

$$\sqrt{\rho_{\boldsymbol{\rho}}} = \|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^2_\xi} \leq \|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}_\lambda\|_{\mathcal{L}^2_\xi} + \|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}^{\mathrm{c}}_\lambda\|_{\mathcal{L}^2_\xi}\,. \tag{63}$$

Now notice that defining $\varphi_\lambda(\xi) = \mathcal{F}\big(\mathbb{1}_{|\xi|^n\leq\lambda}\big)$, the kernel of $\boldsymbol{\chi}_\lambda$ is given by $\boldsymbol{\chi}_\lambda(x,y) = \varphi_{\lambda/h^n}(y-x)$. Therefore

$$(\boldsymbol{\chi}_\lambda\,\boldsymbol{\rho}\,\boldsymbol{\chi}_\lambda)(x,x) = \iint_{\mathbb{R}^{2d}} \varphi_{\frac{\lambda}{h^n}}(y-x)\,\boldsymbol{\rho}(y,z)\,\varphi_{\frac{\lambda}{h^n}}(x-z)\,\mathrm{d}y\,\mathrm{d}z \leq \left\|\varphi_{\frac{\lambda}{h^n}}\right\|_{L^2}^2 \|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}$$

and since by Plancherel theorem $\left\|\varphi_{\frac{\lambda}{h^n}}\right\|_{L^2}^2 = \left\|\mathbb{1}_{|x|\leq\frac{\lambda^{1/n}}{h}}\right\|_{L^2}^2 = \frac{\omega_d}{d}\,\frac{\lambda^{d/n}}{h^d}$, the first term in the right-hand side of Inequality (63) is bounded by

$$\|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}_\lambda\|_{\mathcal{L}^2_\xi}^2 \leq \tfrac{\omega_d}{d}\,\lambda^{d/n}\,\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} =: C_{\boldsymbol{\rho}}^2\,\lambda^{d/n}.$$

We deduce that

$$\left(\sqrt{\rho_{\boldsymbol{\rho}}} - C_{\boldsymbol{\rho}}\,\lambda^{\frac{d}{2n}}\right)_+^2 \leq \|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}_\lambda^{\mathrm{c}}\|_{\mathcal{L}^2_\xi}^2.$$

Now notice that integrating in λ the right-hand side gives

$$\int_0^\infty \left(\sqrt{\rho_{\boldsymbol{\rho}}} - C_{\boldsymbol{\rho}}\,\lambda^{\frac{d}{2n}}\right)_+^2 \mathrm{d}\lambda = c_{d,n}\,C_{\boldsymbol{\rho}}^{-2n/d}\,\rho_{\boldsymbol{\rho}}^{1+n/d}$$

and so since $p = 1 + n/d$, integrating in x gives

$$\begin{aligned} c_{d,n}\,C_{\boldsymbol{\rho}}^{-2n/d} \int_{\mathbb{R}^d} \rho_{\boldsymbol{\rho}}^p &\leq \int_0^\infty\!\!\int_{\mathbb{R}^d} \|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}_\lambda^{\mathrm{c}}\|_{\mathcal{L}^2_\xi}^2\,\mathrm{d}x\,\mathrm{d}\lambda = \int_0^\infty \|\sqrt{\boldsymbol{\rho}}\,\boldsymbol{\chi}_\lambda^{\mathrm{c}}\|_{\mathcal{L}^2}^2\,\mathrm{d}\lambda \\ &\leq \int_0^\infty h^d\,\mathrm{Tr}(\boldsymbol{\rho}\,\chi_\lambda)\,\mathrm{d}\lambda = h^d\,\mathrm{Tr}(\boldsymbol{\rho}\,|\boldsymbol{p}|^n) \end{aligned}$$

which gives the result. □

5.7.2 The Lieb–Thirring inequality

The inequality which is usually called the Lieb–Thirring inequality is the following inequality initially proved in [LT76] for $n = 2$. We recall that $\lambda_j(H)$ denotes the j^{th} eigenvalue of a compact positive operator H, with the eigenvalues ordered in decreasing order of their norm, and $u_- = \max(0, -u)$.

Theorem 5.23 (Lieb–Thirring inequality)**.** *Let $d \geq 1$. Then for any $s \geq 0$ such that $s > 1 - \frac{d}{n}$, there exists an constant $\mathcal{L}_{s,d,n}$ depending only on s, d and n such that the following bound holds*

$$\sum_j \left|\lambda_j\big(((-\Delta)^{\frac{n}{2}} + \mathcal{V})_-\big)\right|^s \leq \frac{\mathcal{L}_{s,d,n}}{(2\pi)^d} \int_{\mathbb{R}^d} \mathcal{V}_-^{s+\frac{d}{n}}. \tag{64}$$

To understand what should be the analogous inequality when $h \to 0$, one can write

$$\sum_j \left|\lambda_j\big(((-\Delta)^{\frac{n}{2}} + \mathcal{V})_-\big)\right|^s = \mathrm{Tr}\Big(\big(-\Delta^{\frac{n}{2}} + \mathcal{V}\big)_-^s\Big) = \frac{(2\pi)^{ns}}{h^{d+ns}} \left\|(|\boldsymbol{p}|^n + \hbar^n\mathcal{V})_-\right\|_{\mathcal{L}^s}^s$$

and so the above inequality can be written with $V = \hbar^n\mathcal{V}$

$$\left\|(|\boldsymbol{p}|^n + V(x))_-\right\|_{\mathcal{L}^s}^s \leq \mathcal{L}_{s,d,n} \int_{\mathbb{R}^d} V_-^{s+\frac{d}{n}}.$$

Hence the analogous inequality in the kinetic setting is

$$I_V := \iint_{\mathbb{R}^{2d}} (|\xi|^n + V)_-^s \, \mathrm{d}x \, \mathrm{d}\xi \leq L_{s,d,n} \int_{\mathbb{R}^d} V_-^{s+\frac{d}{n}} .$$

Notice now that for $V > 0$, by a simple change of variable, one obtains

$$I_V = \int_{\mathbb{R}^d} (V_- - |\xi|^n)_+^s \, \mathrm{d}\xi = V_-^{s+\frac{d}{n}} \, \omega_d \int_0^1 (1 - r^n)^s \, r^{d-1} \, \mathrm{d}r .$$

The last integral can be computed by a formula for the Beta function. Hence in the classical case there is an **equality**

$$\iint_{\mathbb{R}^{2d}} (|\xi|^n + V(x))_-^s \, \mathrm{d}x \, \mathrm{d}\xi = L_{s,d,n} \int_{\mathbb{R}^d} V_-^{s+\frac{d}{n}} = L_{s,d,n} \int_{\mathbb{R}^d} V_-^{p'} , \tag{65}$$

with $p' = s + d/n$ and

$$L_{s,d,n} = \frac{\omega_d}{n} \frac{\Gamma(s+1) \, \Gamma(\frac{d}{n})}{\Gamma(s + \frac{d}{n} + 1)} = \frac{2 \, \omega_d \, \omega_{2(1+p')}}{n \, \omega_{2(s+1)} \, \omega_{2(p'-s)}} . \tag{66}$$

In the particular case when $n = 2$ then $L_{s,d} = \frac{\Gamma(s+1) \, \pi^{d/2}}{\Gamma(s+\frac{d}{2}+1)}$. In the particular case when $d = 3$ and $s = 1$, then $L_{1,3} = \frac{8\,\pi}{15}$.

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