8. "Quantum phase space": Wigner transform and Weyl quantization

8.1. Definition: For $\phi, \psi \in L^2(\mathbb{R}^d)$,

we define the corresponding *Wigner-Function* $W[\phi,\psi]: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$,

$$W[\phi,\psi](x,k) := \int_{\mathbb{R}^d} dy\, e^{-i2\pi k\cdot y}\, \phi\left(x-\frac{y}{2}\right)^* \psi\left(x+\frac{y}{2}\right).$$

The Wigner function of $\psi \in L^2(\mathbb{R}^d)$ is $W[\psi] := W[\psi,\psi]$.

8.2 Proposition (Basic properties) $\forall \phi,\psi \in L^2$:

a) (symmetry) $W[\phi,\psi]^* = W[\psi,\phi]$
b) (reality) $W[\psi](x,k) \in \mathbb{R}\ \forall x,k$.
c) (boundedness) $|W[\phi,\psi](x,k)| \le 2^d \|\phi\|\,\|\psi\|\ \forall x,k$.
d) (Fourier representation) If $\hat{\psi} = \mathcal{F}\psi$ and $\hat{\phi} = \mathcal{F}\phi$, then $\forall\ x,k \in \mathbb{R}^d$

$$W[\phi,\psi](x,k) = W[\hat{\phi},\hat{\psi}](k,-x)$$

$$= \int dq\, e^{+i2\pi q\cdot x}\, \hat{\phi}\left(k-\frac{q}{2}\right)^* \hat{\psi}\left(k+\frac{q}{2}\right)$$

e) (recovery of inner products)
If $\psi,\phi \in \mathcal{S}$, then $W[\phi,\psi] \in \mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$ and

$$\int_{\mathbb{R}^d} dk\, W[\phi,\psi](x,k) = \phi(x)^*\psi(x) \quad \forall x \in \mathbb{R}^d$$

$$\int_{\mathbb{R}^d} dx\, W[\phi,\psi](x,k) = \hat{\phi}(k)^*\hat{\psi}(k) \quad \forall k \in \mathbb{R}^d$$

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} dx\,dk\, W[\phi,\psi](x,k) = (\phi,\psi)$$

f) ("marginals") If $\psi \in S_d$, then $W[\psi] \in S_{2d}$

$$\int dk\, W[\psi](x,k) = |\psi(x)|^2 \quad \forall x$$

$$\int dx\, W[\psi](x,k) = |\hat{\psi}(k)|^2 \quad \forall k$$

$$\int dx\, dk\, W[\psi](x,k) = \|\psi\|_{L^2}^2$$

The results in c) and f) are true also for general $\phi, \psi \in L^2$, if understood in somewhat weaker sense. For instance,

$$\lim_{\varepsilon \to 0} \int dx\, dk\, e^{-\frac{1}{2}\varepsilon^2(x^2+k^2)} W[\phi,\psi](x,k) = (\phi,\psi) \quad \forall \phi,\psi \in L^2.$$

Proof. Obviously, b) follows from a) and f) from e). Thus it suffices to study $W(x,k) := W[\phi,\psi](x,k)$ for fixed $\psi, \phi \in L^2(\mathbb{R}^d)$. Then

$$W(x,k)^* = \int dy\, e^{i2\pi k\cdot y} \psi(x+\tfrac{y}{2})^* \phi(x-\tfrac{y}{2}) \underset{y'=-y}{=} W[\psi,\phi](x,k).$$

This proves a) and b).

$$|W(x,k)| \le \int dy\, |\phi(x+\tfrac{y}{2})|\, |\psi(x-\tfrac{y}{2})|$$

$$\le \sqrt{\int dy\, |\phi(x+\tfrac{y}{2})|^2 \int dy\, |\psi(x-\tfrac{y}{2})|^2}$$

$$= 2^d \|\phi\|\, \|\psi\| \quad \Rightarrow \quad c).$$

To prove d), let us first consider the case $\phi \in L^2$, $\psi \in S_d$. Then, using $z = x - \frac{y}{2}$,

$$W(x,k) = 2^d \int_{\mathbb{R}^d} dz\, e^{-i2\pi k\cdot 2(x-z)} \phi(z)^* \psi(2x-z)$$

where we can use unitarity of $\mathcal{F}_{L^2}$ and the fact that $z \mapsto e^{-i2\pi k\cdot 2(x-z)}\psi(2x-z)$ is a Schwartz function. This proves

$$W(x,k) = 2^d \int_{\mathbb{R}^d} dk'\, \hat{\phi}(k')^* \Big[\int dz\, e^{-i2\pi z\cdot k'} \times e^{-i2\pi(2k\cdot x - 2k\cdot z)} \psi(2x-z) \Big]$$

where $[\,] \overset{y'=2x-z}{=} \int dy'\, e^{-i2\pi y'\cdot(2k-k')}\psi(y') \times e^{i2\pi 2x\cdot(k-k')}$

$$= e^{2\pi x\cdot 2(k-k')}\hat{\psi}(2k-k').$$

Then we let $q = 2(k-k') \Rightarrow k' = k - \frac{q}{2}$

$$W(x,k) = \int_{\mathbb{R}^d} dq\, e^{i2\pi x\cdot q}\, \hat{\phi}(k-\tfrac{q}{2})^* \hat{\psi}(k+\tfrac{q}{2})$$

$$= W[\hat{\phi},\hat{\psi}](k,-x).$$

Thus d) holds, if $\psi \in \mathcal{S}$. For a general $\psi \in L^2$, there is $f_n \in \mathcal{S}$ s.t. $\|\psi - f_n\| \to 0$. Then, since W is linear in ψ,

$$W[\hat{\phi},\hat{\psi}](k,-x)$$
$$= \underbrace{W[\hat{\phi},\hat{\psi}-\hat{f}_n](k,-x)}_{} + W[\hat{\phi},\hat{f}_n](k,-x)$$

$$|\cdot| \le 2^d \|\hat{\phi}\|\,\|\hat{\psi}-\hat{f}_n\| = 2^d\|\phi\|\,\|\psi-f_n\| \xrightarrow{n\to\infty} 0.$$

$$\text{and } W[\hat{\phi},\hat{f}_n](k,-x) = W[\phi,f_n](x,k)$$
$$= W[\phi,\psi](x,k) + \underbrace{W[\phi,f_n-\psi](x,k)}_{\xrightarrow{n\to\infty} 0 \text{ by c)}}$$

Thus d) holds for all $\psi \in L^2$.

For e), assume $\phi,\psi \in \mathcal{S}$. We skip the estimates which prove that then $W[\phi,\psi] \in \mathcal{S}_{2d}$. (one only needs to prove that any differentiation can be done inside the integral, and use the Leibniz rule.). Then all the integrals on the left hand side of e) are well-def. (absolutely convergent). The map

$$x_\pm = x \pm \frac{y}{2} \Rightarrow x^\alpha = 2^{-|\alpha|}(2x)^\alpha = 2^{-|\alpha|}(x_+ + x_-)^\alpha = 2^{-|\alpha|}\sum_{\beta\le\alpha}\binom{\alpha}{\beta} x_+^{\alpha-\beta}x_-^\beta$$

$F_x: y \mapsto \phi(x-\frac{y}{2})^* \psi(x+\frac{y}{2})$ is Schwartz for any x.

Thus by the inversion formula

$$\int dk\left[\int dy\, F_x(y)\, e^{-i2\pi k\cdot y}\right] = \int dk\, \hat{F}_x(k)$$
$$= F_x(0) = \phi(x)^*\psi(x).$$

Then d) shows that $\int dx\, W(x,k) = \int dx\, W[\hat\phi,\hat\psi](k,-x)$
$= \int dx'\, W[\hat\phi,\hat\psi](k,x') = \hat\phi(k)^*\hat\psi(k)$,
since $\hat\phi,\hat\psi \in S_d$. Therefore, by Fubini,

$$\int dx\, dk\, W[\phi,\psi](x,k) = \int dx\left(\int dk\, W[\phi,\psi](x,k)\right)$$
$$= \int dx\, \phi(x)^*\psi(x) = (\phi,\psi).$$

These results prove e) & f) $\square$

8.3. Application I: Scaling limits

3.1. Definition: The Wigner function on spatial scale ε^{-1}, $\varepsilon>0$, is defined by

$$W^\varepsilon[\phi,\psi](x,k) := \varepsilon^{-d} W[\phi,\psi](\tfrac{x}{\varepsilon},k)$$

$$\overset{8.2.d)}{\Rightarrow} W^\varepsilon[\phi,\psi](x,k) = \int dq\, e^{i2\pi q\cdot x}\hat\phi(k-\varepsilon\tfrac{q}{2})^*\hat\psi(k+\varepsilon\tfrac{q}{2}).$$

3.2. Definition: The Wigner transform of $\psi \in L^2(\mathbb{R}^d)$ is the map

$$W_\psi : S(\mathbb{R}^d\times\mathbb{R}^d) \to \mathbb{C} \quad \text{defined by}$$

$$W_\psi(f) := \int dx\, dk\, W[\psi](x,k)\, f(x,k)$$

Similarly, the rescaled Wigner transform is

$$W^\varepsilon_\psi(f) := \int dx\, dk\, W^\varepsilon[\psi](x,k)\, f(x,k)$$
$$= \int dy\, dk\, W[\psi](y,k)\, f(\varepsilon y,k).$$

Interlude:

7. Distribution theory on $\mathbb{R}^d$: crash course on basic results

7.1. Let $\Omega \subset \mathbb{R}^d$ be open and non-empty. Consider the following function space:

$$C_c^\infty(\Omega) := \{ f : \Omega \to \mathbb{C} \mid f \text{ smooth and } \operatorname{supp} f := \overline{\{x \mid f(x) \neq 0\}}^{\Omega} \text{ compact} \}$$

1. Proposition: We can define a topology $\tau_{\mathcal{D}}$ on $C_c^\infty(\Omega)$

(a locally convex vector topology) such that a linear map $\Lambda : C_c^\infty(\Omega) \to \mathbb{C}$ is continuous if and only if it satisfies:

($\mathcal{D}'$-cond.) If $K \subset \Omega$ is compact, then there is $N_K \in \mathbb{N}_0$ and $C_K < \infty$ such that

$$|\Lambda(f)| \leq C_K \sup \{ |\partial^\alpha f(x)| \mid x \in \Omega, |\alpha| \leq N_K \},$$

for any f with $\operatorname{supp} f \subset K$.

Proof: Rudin, F.A., section 6.2. $\square$

2. Definition The space $C_c^\infty(\Omega)$ with topology $\tau_{\mathcal{D}}$ is called the space of compactly supported test-functions, and denoted by $\mathcal{D}(\Omega)$. Its dual is denoted by

$$\mathcal{D}'(\Omega) := \{ \Lambda : \mathcal{D}(\Omega) \to \mathbb{C} \mid \Lambda \text{ linear and continuous} \}.$$

$\Lambda \in \mathcal{D}'(\Omega)$ is called an (ordinary) distribution on Ω.

Unless stated otherwise, $\mathcal{D}'(\Omega)$ is endowed with its "weak-$*$" topology, which is the weakest topology, for which the maps $\Lambda \mapsto \Lambda(f)$ are continuous for any fixed f.

3. Proposition (Basic properties)

a) For any multi-index α, the map $f \mapsto \partial^\alpha f$ is continuous, $\mathcal{D}(\Omega) \to \mathcal{D}(\Omega)$.

b) If $\Lambda \in \mathcal{D}'(\Omega)$ and α is a multi-index, the map $f \mapsto (-1)^{|\alpha|} \Lambda(\partial^\alpha f)$ is a distribution, denoted by $\partial^\alpha \Lambda$.

c) If $\Lambda(f) \geq 0$ for all $f \in \mathcal{D}(\Omega)$ with $f \geq 0$, then there is a unique positive Radon measure μ_Λ on Ω such that

$$\Lambda(f) = \int_\Omega \mu_\Lambda(dx)\, f(x) \quad \forall f \in \mathcal{D}(\Omega).$$

Proof: a) = Rudin, FA, Thrm 6.6.
b) follows from a).
c) = Lieb, Loss, Analysis, Thrm 6.22. □

4. The topology τ_D is somewhat unpleasant, it is non-metrizable, for instance. It is, however, complete, and leads to the following extremely nice property for convergence of a sequence of distributions:

Proposition: Suppose $\Lambda_n \in \mathcal{D}'(\Omega)$ $\forall n = 1, 2, \ldots,$

and for all $f \in \mathcal{D}(\Omega)$:

$$\exists \tilde{\Lambda}_f := \lim_{n \to \infty} \Lambda_n(f). \quad (\text{in } \mathbb{C})$$

then a) The map $\Lambda : f \mapsto \tilde{\Lambda}_f$ is a distribution, and $\Lambda_n \to \Lambda$.

b) $\forall$ multi-index α

$$\partial^\alpha \Lambda_n \to \partial^\alpha \Lambda \quad (\text{in the topology of } \mathcal{D}'(\Omega)).$$

Proof Rudin, FA, 6.17. □

7.2. Tempered distributions = Schwartz distributions

Consider then $\Omega = \mathbb{R}^d$, and denote
$\mathcal{D}_d := \mathcal{D}(\mathbb{R}^d)$, $\mathcal{D}'_d = \mathcal{D}'(\mathbb{R}^d)$
and recall the definition of the Schwartz space S_d in Sect. 6.2. (also its topology).

The dual of S_d is called the space of tempered distributions, and it is denoted by

$$S'_d := \{ \Lambda : S_d \to \mathbb{C} \mid \Lambda \text{ linear and continuous} \}.$$

Clearly, $\mathcal{D}_d \subset S_d$. Moreover, $\mathcal{D}_d$ is dense in S_d and the map $J(f) = f$ is continuous $\mathcal{D}_d \to S_d$ (Rudin, FA, theorem 7.10.). Thus for any $\Lambda \in S'_d$, $\Lambda \circ J \in \mathcal{D}'_d$, and $\Lambda \circ J$ is an ordinary distribution. In addition, if $\Lambda \circ J = \Gamma$ for some $\Gamma \in \mathcal{D}'_d$, then $\Lambda|_{\mathcal{D}} = \Gamma$ $\Rightarrow \Lambda = \overline{\Gamma}$ since $\mathcal{D}$ is dense in S. Thus we can identify S'_d with

$$\mathcal{D}^{\text{Temp.}}_d := \{ \Gamma \in \mathcal{D}'(\mathbb{R}^d) \mid \Gamma \text{ has a continuous extension to } S_d \},$$

which is a subspace of $\mathcal{D}'_d$.

1. →

2. Tempered distributions are nice since they can be studied via the Fourier transform:

Definition: For any $\Lambda \in S'_d$ we define

$$\hat{\Lambda}(f) := \Lambda(\underbrace{\mathcal{F}f}_{\in S_d!}) \quad \forall f \in S_d.$$

3. Proposition

a) $\forall \Lambda \in \mathcal{S}'$ also $\hat{\Lambda} \in \mathcal{S}'$.

b) The map $\mathcal{F}_{\mathcal{S}'} : \Lambda \mapsto \hat{\Lambda}$ is a continuous, linear bijection $\mathcal{S}'_d \to \mathcal{S}'_d$. In addition,

$\mathcal{F}_{\mathcal{S}'}^4 = \mathrm{id}$ and the inverse of $\mathcal{F}_{\mathcal{S}'}$ is also continuous.

c) For any multi-index α, and $\Lambda \in \mathcal{S}'$, $\partial^\alpha \Lambda$ and $x^\alpha \Lambda \in \mathcal{S}'$.

Proof. a, b) = Rudin, FA, Thm. 7.15.
c) = Rudin, FA, Thm. 7.13. □

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1. Proposition A linear map $\Lambda : \mathcal{S}_d \to \mathbb{C}$

is continuous if and only if $\exists N \in \mathbb{N}_0$ and $C < \infty$ such that

$$|\Lambda(f)| \le C \|f\|_{\mathcal{S},N} \quad \forall f \in \mathcal{S}_d.$$

Proof. Rudin, FA, Exercise 8. on p. 37, in chapter 1. □

Then back to Wigner...

8.3.3. Theorem: For any $\psi \in L^2(\mathbb{R}^d)$ and $\varepsilon > 0$, W_ψ and W_ψ^ε are tempered distributions.

Proof: By 8.2.c) and the definition 8.3.2.

$$|W_\psi(f)| \leq \int dx\, dk\, |f(x,k)| \cdot 2^d \|\psi\|_{L^2}^2 = 2^d \|\psi\|_{L^2}^2 \|f\|_{L^1}$$

As on p. 66, we have here

$$\|f\|_{L^1} \leq \sup_{y \in \mathbb{R}^{2d}} \left[(1+y^2)^{2d} |f(y)|\right] \cdot \underbrace{\int_{\mathbb{R}^{2d}} dy\, (1+y^2)^{-2d}}_{<\infty}$$

$$\leq C \|f\|_{S,4d}$$

therefore, there is a constant C_d, which depends only on d, such that

(*) $$|W_\psi(f)| \leq C_d \|\psi\|_{L^2}^2 \|f\|_{S,4d} < \infty \quad \forall f \in S_{2d}.$$

In particular, the integral defining W_ψ is absolutely convergent. Since the map $f \mapsto W_\psi(f)$ is clearly linear, (*) allows using 7.2.1. to conclude that W_ψ is a tempered distribution.

By the definition 8.3.1. we then also have

$$W_\psi^\varepsilon(f) = \int dx\, dk\, \varepsilon^{-d} w[\psi]\left(\tfrac{x}{\varepsilon}, k\right) f(x,k)$$

as above

$\Rightarrow$ W_ψ^ε linear and satisfies

$$|W_\psi^\varepsilon(f)| \leq \varepsilon^{-d} 2^d \|\psi\|_{L^2}^2 \|f\|_{L^1}$$

$\Rightarrow W_\psi^\varepsilon \in S_{2d}'$. $\square$

3.4. Remarks The terms "Wigner-function" and "transform" are often used to denote both the above function and the corresponding distribution. The scaling factor in the definition of W^ε is chosen so that $\forall \psi \in \mathcal{S}$, $\varepsilon > 0$

$$\int dx\, dk\; W^\varepsilon[\psi](x,k) = \|\psi\|^2 .$$

The idea behind the scaling is to study large scale variation of ψ or ψ^ε by considering the limit $\varepsilon \to 0$. As the following theorem shows, in these limits the Wigner transform of a wave function becomes a true probability measure on the phase space $\mathbb{R}^d \times \mathbb{R}^d$:

3.5. Theorem Suppose $\varepsilon_n > 0$, $n = 1, 2, \ldots$, is a sequence for which $\varepsilon_n \xrightarrow{n\to\infty} 0$. Let also (ψ_n) be a sequence in $L^2(\mathbb{R}^d)$ such that $\|\psi_n\| = 1$ $\forall n$ and

$$\exists \lim_{n\to\infty} W^{\varepsilon_n}_{\psi_n}(f) =: W^0(f), \quad \forall f \in \mathcal{S}.$$

Then there is a positive Radon measure μ^0 on $\mathbb{R}^d \times \mathbb{R}^d$ s.t. $\int \mu^0(dx\, dk) \le 1$ and

$$W^0(f) = \int \mu^0(dx\, dk)\, f(x,k) \quad \forall f \in \mathcal{S}.$$

In addition, if (ψ_n) is also "tight on the scale ε_n^{-1}" and "have bounded oscillations" then $\int \mu^0(dx\, dk) = 1$ and μ^0 is thus a probability measure on $\mathbb{R}^d \times \mathbb{R}^d$.

Proof. Idea is to prove that W^0 is positive. For details, see for instance Proposition 1.7. in Gérard, et al., Comm. Pure Appl. Math. Vol. 50, pp. 323-379 (1997). [Link on the course webpage].

The extra conditions for (ψ_n) are explicitly:

$$\varepsilon^{-1}\text{-tightness}: \quad \limsup_{n\to\infty} \int_{|x|\geq \frac{R}{\varepsilon_n}} dx\, |\psi_n(x)|^2 \xrightarrow{R\to\infty} 0$$

"bounded oscillations" = "$(\hat{\psi}_n)$ tight"

$$\Leftrightarrow \limsup_{n\to\infty} \int_{|x|\geq R} dx\, |\hat{\psi}_n(x)|^2 \xrightarrow{R\to\infty} 0. \qquad \square$$

<u>3.6. Remark</u> Typical application is to study

$$\psi_n = \psi_n(t) := e^{-i\frac{t}{\varepsilon_n}H}\psi_n(0) \quad .$$

"kinetic" scaling

$t \sim \varepsilon_n^{-1}, \quad x \sim \varepsilon_n^{-1}$

or to study "semi-classical" limits: potential V^{ε_n} is defined by $V^{\varepsilon_n}(x) = V(\varepsilon_n x)$.

For free evolution, the evolution of the Wigner transform is remarkably simple:

<u>3.7. Theorem</u> For any $\psi_0 \in L^2$, $t\in\mathbb{R}$; let

$$\Lambda_t := W_{\psi(t)}, \quad \text{where } \psi(t) = e^{-itH_0}\psi_0$$

is the solution to the free Schrödinger evolution with initial data ψ_0. Then

$$\partial_t \Lambda_t(x,k) + 2\pi k\cdot\nabla_x \Lambda_t(x,k) = 0,$$

meaning that $\forall f\in\mathcal{S}$

$$\partial_t \Lambda_t(f) + \Lambda_t\left(-2\pi k\cdot\nabla_x f(x,k)\right) = 0.$$

<u>Proof</u>: Exercise 9.4. $\square$