LECTURE 15: L^2-THEORY OF SEMICLASSICAL PsDOs: POSITIVITY

1. The weak Gårding inequality

¶ Positivity: a counterexample.

The last "quantitative aspect" of the quantization procedure $a \rightsquigarrow \widehat{a}^W$ we want to study is the positivity: If a is positive (and thus real-valued), what kinds of "positivity" does the operator $\widehat{a}^W$ admit? Is it always a positive operator? Here we only use the Weyl quantization, since other t-quantization will not convert real-valued functions to self-adjoint operators in general.

Recall that a densely defined symmetric A is called *positive* if

$$\langle Au, u\rangle \geq 0, \quad \forall u \in D(A).$$

For example, for any densely defined closed operator A, the operator A^*A is always a positive operator. As usual we will use the notation $A \geq 0$ if A is a positive operator, and use the notation $A \geq B$ if A, B are densely-defined symmetric operators and $A - B$ is a positive operator. It is not hard to prove A is positive if and only if $A = B^2$ for some positive self-adjoint operator B. Equivalently, by the spectral theorem, a self-adjoint linear operator A is positive if and only if $\mathrm{Spec}(A) \subset [0, +\infty)$.

To study the relation between positivity of operators and of corresponding symbols, let's start with two simple examples, which tells us that the positive operator need not have nonnegative symbol, and conversely, the Weyl quantization of a nonnegative function need not be a positive operator:[1]

Similarly we can prove that it is possible that a is not nonnegative while $\widehat{a}^W$ is positive:

The first example is simple: Consider $a(x,\xi) = x^2 + \xi^2 - \hbar$. Then

$$\widehat{a}^W = Q^2 + P^2 - \hbar.$$

According to our result for the quantum harmonic oscillator (Lecture 3), $\widehat{a}^W$ is a positive operator, but its symbol a is not a non-negative function.

[1] In general, we call a quantization procedure a *positive quantization* if it sends nonnegative-valued functions to positive operators. So the Weyl quantization (and in fact any t-quantization) is not a positive quantization. The so-called anti-Wick quantization (also known as Berezin-Toeplitz quantization) is a positive quantization.

The other direction is a bit more complicated. Let $a(x,\xi) = x^2\xi^2$. Then by McCoy's formula (Lecture 7),

$$\widehat{a}^W = \frac{1}{4}(P^2Q^2 + 2QP^2Q + Q^2P^2).$$

If we let $b(x,\xi) = x\xi$, then $\widehat{b}^W = \frac{1}{2}(QP + PQ)$, which implies

$$\begin{aligned}(\widehat{b}^W)^2 &= \frac{1}{4}(PQPQ + QPQP + QP^2Q + PQ^2P)\\ &= \frac{1}{4}(P^2Q^2 + i\hbar PQ + Q^2P^2 - i\hbar QP + QP^2Q + (QP - i\hbar)(PQ + i\hbar))\\ &= \widehat{a}^W + \frac{1}{4}\hbar^2.\end{aligned}$$

On the other hand, it can be proven that $\mathrm{Spec}((\widehat{b}^W)^2) = [0,+\infty)$. (Formally by solving ODE one can find the function $x^{-1/2}$ which satisfies

$$\widehat{b}^W(x^{-1/2}) = \frac{1}{2}\left[x(-\frac{1}{2})x^{-3/2} + \frac{1}{2}x^{-1/2}\right] = 0.$$

Of course the function $x^{-1/2}$ is far from being in our space. For example, $x^{-1/2}$ is only defined on $(0,+\infty)$. So it is natural to consider the diffeomorphism $\mathbb{R} \to (0,+\infty)$ which sends x to e^x. The diffeomorphism induces a natural unitary operator from $L^2(\mathbb{R})$ to $L^2((0,+\infty))$, sending $f(x)$ to $e^{x/2}f(e^x)$. One can show that this unitary operator will conjugate $\widehat{b}^W$ (restricted to $L^2((0,+\infty))$) to the operator P on $L^2(\mathbb{R})$. It is well-known that the spectrum of the momentum operator P is $\mathbb{R}$. It follows that $\mathrm{Spec}(\widehat{b}^W) = \mathbb{R}$ and thus $\mathrm{Spec}((\widehat{b}^W)^2) = [0,+\infty)$. It follows that

$$\mathrm{Spec}(\widehat{a}^W) = [-\frac{1}{4}\hbar^2, +\infty)$$

and thus $\widehat{a}^W$ is not a positive operator.

¶ Semiclassical Gårding inequality: a simple version.

In the remaining of this lecture, we will show that if a is non-negative, then $\widehat{a}^W$ is "almost positive". We start with a simple version which claims that if $a \geq 0$, then $\widehat{a}^W \geq -\varepsilon \cdot \mathrm{Id}$:

Theorem 1.1 (Weak Gårding inequality)**.** *Suppose $a \in S(1)$ is nonnegative, i.e. $a \geq 0$. Then for any $\varepsilon > 0$, there exists $\hbar_0 > 0$ such that for any $\hbar \in (0,\hbar_0)$,*

$$\langle \widehat{a}^W u, u\rangle \geq -\varepsilon\|u\|^2_{L^2(\mathbb{R}^n)}, \qquad \forall u \in L^2(\mathbb{R}^n).$$

Proof. By definition, for any $\delta < -\varepsilon$, $a - \delta$ is elliptic in $S(1)$. So according to what we learned last time, there exists $\hbar_0 = \hbar_0(\delta)$ such that for any $\hbar \in (0,\hbar_0)$, the operator $\widehat{a}^W - \delta \cdot \mathrm{Id}$ is invertible and the inverse is a bounded linear operator. In what follows we will show:

Claim: Fixing a and ε, the constant $\hbar_0 = \hbar_0(\delta)$ can be chosen to be independent of the choice of $\delta < -\varepsilon$.

As a consequence, the interval $(-\infty, -\epsilon)$ lies in the resolvent set of $\widehat{a}^W$ for any $\hbar \in (0, \hbar_0)$, and thus the spectrum $\mathrm{Spec}(\widehat{a}^W) \subset [-\epsilon, +\infty)$ uniformly for all $\hbar \in (0, \hbar_0)$. By spectral theorem for bounded linear operators, we get $\langle \widehat{a}^W u, u\rangle \geq -\varepsilon \|u\|^2_{L^2(\mathbb{R}^n)}$ for any $\hbar \in (0, \hbar_0)$.

So it remains to prove the claim. For this we have to go back to the proof of the invertibility. According to the remark after Corollary 1.4 in Lecture 14, we it is enough to find $\hbar_0$ so that

$$\|\widehat{r}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} < 1/2, \quad \forall \hbar \in (0, \hbar_0)$$

holds for all $\delta < -\varepsilon$, where

$$r = 1 - (a-\delta) \star \frac{1}{a-\delta}.$$

It is easy to check[2]

$$\{a - \delta, \frac{1}{a-\delta}\} = 0,$$

we have

$$1 - (a - \delta) \star \frac{1}{a-\delta} = O(\hbar^2)$$

According to Calderon-Vaillancourt theorem, we need a uniform estimate of $\|\partial^\alpha r\|_{L^\infty}$ for all $\delta < -\varepsilon$. So we only need to find uniform bound for

$$\|\partial^\alpha (a - \delta)\|_{L^\infty(\mathbb{R}^n)} \quad \text{and} \quad \|\partial^\alpha (\frac{1}{a-\delta})\|_{L^\infty(\mathbb{R}^n)}$$

Since $a \in S(1)$, all derivatives of $a - \delta$ is uniformly bounded. Note: $a - \delta$ itself is NOT bounded. However, we will not need it in computing r. We only need derivatives of $a - \delta$. On the other hand, as in last lecture, by induction one can prove

$$\partial^\alpha (\frac{1}{a-\delta}) = \frac{1}{a-\delta} \sum_{\beta_1+\cdots+\beta_k=\alpha, |\beta_j|\geq 1} C_{\beta_1\cdots\beta_k} \prod_j (\frac{1}{a-\delta} \partial^{\beta_j} a) \tag{1}$$

It follows that for any α, $\|\partial^\alpha(\frac{1}{a-\delta})\|_{L^\infty}$ is uniformly bounded for all $\delta < -\varepsilon$. So there exists a constant C, uniformly for all $\delta < -\varepsilon$, such that

$$\|\widehat{r}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} \leq C\hbar^2$$

and the conclusion follows. □

[2] More general, for any $a(x, \xi)$ and any one-variable function f, one can easily check $\{a(x, \xi), f(a(x, \xi))\} = 0$.

2. The sharp Gårding inequality

¶ Sharp (semiclassical) Gårding inequality.

The weak Gårding inequality is "weak" because the lower bound we get is not "semiclassical small", thus as $\hbar \to 0$ the lower bound could be relatively large. Our main goal in this lecture is to prove the following sharp Gårding inequality, which claims that the Weyl quantization of a nonnegative symbol is "semiclassically close to be positive":

Theorem 2.1 (Sharp Gårding inequality)**.** *Suppose $a \in S(1)$ and $a \geq 0$. Then there exists constant $C \geq 0$ and $\hbar_0 > 0$ such that for all $\hbar \in (0, \hbar_0)$,*

$$\langle \widehat{a}^W u, u\rangle \geq -C\hbar \|u\|^2_{L^2(\mathbb{R}^n)}, \qquad \forall u \in L^2(\mathbb{R}^n).$$

Remark. With more work, one can prove a stronger inequality: the (semiclassical) *Fefferman-Phong inequality*:

$$\langle \widehat{a}^W u, u\rangle \geq C\hbar^2 \|u\|^2_{L^2(\mathbb{R}^n)}, \qquad \forall u \in L^2(\mathbb{R}^n).$$

In view of the examples at the beginning of this lecture, this inequality is sharp.

In Lecture 11, as a consequence of the Calderon-Vaillancourt theorem, we get

$$\|\widehat{a}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} \leq C \sup_{\mathbb{R}^n} |a| + O(\hbar^{1/2}).$$

Now we can remove the constant C by using the Sharp Gårding inequality:

Corollary 2.2. *Suppose $a \in S(1)$. Then*

$$\|\widehat{a}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} \leq \sup_{\mathbb{R}^n} |a| + O(\hbar).$$

Proof. For any $u \in L^2$ with $\|u\|_{L^2} = 1$, we have

$$\|\widehat{a}^W u\|^2_{L^2} = \langle (\widehat{a}^W)^* \widehat{a}^W u, u\rangle_{L^2} = \langle \widehat{\overline{a}}^W \widehat{a}^W u, u\rangle_{L^2}.$$

Since

$$\widehat{\overline{a}}^W \widehat{a}^W = \widehat{|a|^2}^W + O(\hbar),$$

we get from the sharp Gårding inequality

$$\|\widehat{a}^W u\|^2 = \langle \widehat{|a|^2}^W u, u\rangle + O(\hbar) \geq (\sup |a|)^2 + O(\hbar).$$

□

Similarly one can prove: If $a \in S(1)$ is real-valued, then there exists C and $\hbar_0$ such that

$$\inf a - C\hbar \leq \widehat{a}^W \leq \sup a + C\hbar.$$

¶ Proof of Sharp Gårding inequality: First thoughts.

Now we try to prove the Sharp Gårding inequality. Again, it is enough to prove that for $\delta < -C\hbar$, the operator $\widehat{a-\delta}^W$ has a bounded inverse for all $\hbar \in (0, \hbar_0)$. In view of the weak Gårding inequality, We may assume $\delta > -1$ now. Again we want to control the L^∞-norms of partial derivatives of $a-\delta$ and $\frac{1}{a-\delta}$. Again the L^∞-norm of each derivative of $a-\delta$ is uniformly controlled. So the only problem is to get a uniform control of the L^∞-norm of each partial derivative of $\frac{1}{a-\delta}$, which is quite non-trivial now.

We still need to apply the formula (1). Since $a \geq 0$ and $\delta < 0$, we have

$$\|\frac{1}{a-\delta}\|_{L^\infty} \leq \frac{1}{|\delta|}.$$

For partial derivatives, we have a rough bound

$$\|\frac{1}{a-\delta}\partial^{\beta_j} a\|_{L^\infty} \leq C_{\beta_j}\frac{1}{|\delta|}$$

which only give us

$$\|\partial^\alpha \frac{1}{a-\delta}\|_{L^\infty} \leq C_\alpha \frac{1}{a-\delta}\frac{1}{|\delta|^{|\alpha|}}.$$

So under the condition $\delta \in (-1, -C\hbar)$ and $a \geq 0$, we only get

$$\|\partial^\alpha \frac{1}{a-\delta}\|_{L^\infty} \leq \frac{1}{|\delta|} C_\alpha \hbar^{-|\alpha|},$$

i.e. $\frac{\hbar}{a-\delta} \in S_1(1)$, which is a very bad symbol class: Recall that the symbol class $S_\rho(1)$ is almost as nice as $S(1)$ for $\rho \in (0, \frac{1}{2})$, but will be very bad for $\rho > \frac{1}{2}$.

Fortunately, there is a critical symbol class, $S_{1/2}(1)$, which is not as good as $S(1) = S_0(1)$ since we will not have those nice asymptotic expansions as we have explained in Lecture 10, but it is also not that bad in the sense that we can still get many useful results after hard working, e.g. we still have a nice explicit formula for the Moyal product.

To finish the proof of the Sharp Gårding inequality, we first notice that if $|\beta| \geq 2$, then we have (Note: $|\delta| < 1$.)

$$\|\frac{1}{a-\delta}\partial^{\beta_j} a\|_{L^\infty} \leq C_{\beta_j}\frac{1}{|\delta|} \leq C\frac{1}{|\delta|^{|\beta_j|/2}}.$$

So in view of (1), it is possible to improve the symbol class from $S_1(1)$ to $S_{1/2}(1)$ as long as we can prove the same inequality for $|\beta| = 1$. For this purpose we will need to use the following elementary gradient estimate:

¶ DETOUR: A gradient estimate for positive functions.

Before we prove the theorem, we need a couple preparation. Suppose $f \in C^2(\mathbb{R})$ and $f \geq 0$, then by Taylor's expansion, there exists $\tilde{x} \in (x, x+t)$ such that

$$0 \leq f(x+t) = f(x) + tf'(x) + \frac{t^2}{2} f''(\tilde{x}).$$

Thus if $|f''| \leq A$ and if we take $t = -f'/A$ we conclude

$$|f'| \leq \sqrt{2Af}.$$

This simple fact has the following multi-variable generalization,

Lemma 2.3 (Gradient estimate)**.** *Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is non-negative, C^2, and $|\partial^2 f| \leq A$ (meaning $x^T(\partial^2 f)x \leq A|x|^2$ for any $x \in \mathbb{R}^n$). Then*

$$|\nabla f| \leq \sqrt{2Af}.$$

Proof. The proof is almost the same as the one variable case. The only difference is that we use the following Taylor's expansion with integral remainder:

$$0 \leq f(x+t) = f(x) + \langle \nabla f, t\rangle + \int_0^1 (1-s)\langle \partial^2 f(x+st)t, t\rangle ds.$$

Taking $t = -\frac{1}{A}\nabla f(x)$, we get

$$|\nabla f|^2 \leq Af + A^2 \int_0^1 (1-s) ds \cdot \langle t, t\rangle = Af - |\nabla f|^2/2,$$

from which the conclusion follows. □

¶ DETOUR: The critical symbol class $S_{1/2}(m)$.

We also list some results for $S_{1/2}(m)$ that we need. Recall that $a \in S_\delta(m)$ if for any α,

$$|\partial^\alpha a| \leq C_\alpha \hbar^{-\delta|\alpha|} m.$$

We need the following results for the critical symbol class $S_{1/2}(m)$:

(I) For any symmetric non-singular $2n \times 2n$ matrix Q, the operator $\widehat{e^{\frac{i}{2\hbar}\xi^T Q \xi}}^W$ maps $S_{1/2}(m)$ to $S_{1/2}(m)$. (But we will not have the asymptotic expansion as in the case of $\delta < \frac{1}{2}$.)

(II) If $a \in S_{1/2}(m_1), b \in S_{1/2}(m_2)$, then $a \star b \in S_{1/2}(m_1 m_2)$ and

$$a \star b(x,\xi) = \left[e^{\frac{i\hbar}{2}(D_\xi \cdot D_y - D_x \cdot D_\eta)} (a(x,\xi) b(y,\eta)) \right]_{y=x, \eta=\xi}$$

(III) (Calderon-Vaillancourt for critical symbol) For $a \in S_{1/2}(1)$, $\widehat{a}^W$ is bounded on $L^2(\mathbb{R}^n)$ and

$$\|\widehat{a}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} \leq C \sum_{|\alpha| \leq Mn} \hbar^{|\alpha|/2} \|\partial^\alpha a\|_{L^\infty(\mathbb{R}^n)}.$$

We will only prove (I), since the proofs to (II) and (III) will be similar to earlier proofs.

Proof of (I).

We re-scale by setting $\widetilde{w} = \hbar^{-1/2}w$. Then

$$\begin{aligned} e^{\frac{i}{2\hbar}\zeta^T Q\zeta}a(z) &= \frac{C}{\hbar^n}\int_{\mathbb{R}^{2n}} e^{-\frac{i}{2\hbar}p_{Q^{-1}}(w)}a(z+w)dw \\ &= C\int_{\mathbb{R}^{2n}} e^{-\frac{i}{2}p_{Q^{-1}}(\widetilde{w})}a(z+\hbar^{1/2}\widetilde{w})d\widetilde{w} \\ &= C\int_{\mathbb{R}^{2n}} e^{-\frac{i}{2}p_{Q^{-1}}(\widetilde{w})}a(z+\hbar^{1/2}\widetilde{w})\chi_1(\tilde{w})d\widetilde{w} + C\int_{\mathbb{R}^{2n}} e^{-\frac{i}{2}p_{Q^{-1}}(\widetilde{w})}a(z+\hbar^{1/2}\widetilde{w})(1-\chi_1(\widetilde{w}))d\widetilde{w}, \end{aligned}$$

where χ_1 is a compactly supported cut-off function which equals 1 near the origin. For the first part, one has

$$\left|\partial_z^\alpha \int_{\mathbb{R}^{2n}} e^{-\frac{i}{2}p_{Q^{-1}}(\tilde{w})}a(z+\hbar^{1/2}\tilde{w})\chi_1(\tilde{w})d\tilde{w}\right| \le C\hbar^{-|\alpha|/2}m(z),$$

and for the second part, one use an integration by parts argument via $L = \frac{\nabla p_{Q^{-1}}\cdot \hbar D}{|\nabla p_{Q^{-1}}|^2}$ as we did in proving non-stationary phase. □

¶ Proof of Sharp Gårding inequality: continued.

We have mentioned that for $|\beta_j| \ge 2$, we have

$$\|\frac{1}{a-\delta}\partial^{\beta_j}a\|_{L^\infty} \le C_{\beta_j}\frac{1}{|\delta|} \le C\frac{1}{|\delta|^{|\beta_j|/2}}.$$

For $|\beta_j| = 1$ we use the gradient estimate to get

$$|\nabla a| \le C\sqrt{a} \le C\frac{a-\delta}{\sqrt{|\delta|}}$$

and thus

$$\|\frac{1}{a-\delta}\partial^{\beta_j}a\|_{L^\infty} \le C\frac{1}{\sqrt{|\delta|}}.$$

Combining these two cases together, we conclude that for any α,

$$\|\partial^\alpha\frac{1}{a-\delta}\|_{L^\infty} \le C_\alpha\frac{1}{a-\delta}|\delta|^{-|\alpha|/2}.$$

Now we for $\delta \in (-1, -C\hbar)$, we write $\delta = -\hbar/\tilde{\hbar}$. So $\tilde{h} \in (\hbar, \frac{1}{C})$. Since $\frac{1}{a-\delta} \le \frac{1}{-\delta}$, we can rewrite the above inequality as

$$\|\partial^\alpha\frac{\hbar}{a-\delta}\|_{L^\infty} \le C_\alpha\tilde{\hbar}\cdot\hbar^{-|\alpha|/2},$$

i.e. $\frac{\hbar}{a-\delta} \in \tilde{\hbar}S_{1/2}(1)$, Since $a-\delta \in S(1) \subset S_{1/2}(1)$ and $\frac{\hbar}{a-\delta} \in \tilde{\hbar}S_{1/2}(1)$, the Moyal star product $(a-\delta)\star\frac{1}{a-\delta}$ is given by the above formula. To get an explicit expression, we notice that for any one-variable smooth function f, one has

$$f(1) = f(0) + f'(0) + \int_0^1 (1-s)f''(s)ds$$

Apply this to

$$f(t) = \left[e^{\frac{it\hbar}{2}(D_\xi\cdot D_y - D_x\cdot D_\eta)}((a(x,\xi)-\delta)\frac{1}{a(y,\eta)-\delta})\right]_{y=x,\eta=\xi}$$

and notice

$$f'(0) = \frac{i\hbar}{2}(D_\xi\cdot D_y - D_x\cdot D_\eta)\left[(a(x,\xi)-\delta)\frac{1}{a(y,\eta)-\delta}\right]_{y=x,\eta=\xi} = \frac{i\hbar}{2}\{a-\delta, \frac{1}{a-\delta}\} = 0$$

we get

$$(a-\delta)\star\frac{1}{a-\delta} = 1+\int_0^1 (1-s)\left[e^{\frac{is\hbar}{2}(D_\xi\cdot D_y - D_x\cdot D_\eta)}\left(\frac{i\hbar}{2}(D_\xi\cdot D_y - D_x\cdot D_\eta)\right)^2 (a(x,\xi)b(y,\eta))\right]_{y=x,\eta=\xi} ds$$

Finally as in the proof of the weak Gårding inequality, we denote

$$r(x,\xi) = 1-(a-\delta)\star\frac{1}{a-\delta}.$$

We want to prove $\|\widehat{r}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} < \frac{1}{2}$ uniformly for $\hbar < \hbar_0$ and $\delta \in (-\varepsilon, -1)$.

Observe that $\frac{\hbar}{a-\delta} \in \tilde{\hbar}S_{1/2}(1)$ implies $\hbar^2\partial^\alpha(\frac{1}{a-\delta}) \in \tilde{\hbar}S_{1/2}$ for any $|\alpha| = 2$. This together with (I) implies $r \in \tilde{\hbar}S_{1/2}(1)$. So by (III),

$$\|\widehat{r}^W\|_{\mathcal{L}(L^2(\mathbb{R}^n))} \le C_1\tilde{\hbar}.$$

So if we take C large enough, we can get $C_1/C < 1/2$. The conclusion follows.