Radboud University

Master's Thesis

Semiclassical analysis

the double well potential in the semiclassical limit

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Abstract

Semiclassical analysis deals with the relationship between classical dynamics and the behaviour of solutions to pseudodifferential operators depending on a small parameter $h > 0$. Let $a : \mathbb{R}^{2n} \to \mathbb{C}$ be a function, then we can associate it with an operator $a^W(x, hD)$. In the context of quantum mechanics, taking the limit $h \to 0$ is a way to study the classical limit of quantum mechanics. In the first part of this thesis, we will follow [8] and prove the Agmon-Lithner estimate and the Carleman inequality.

The second part of this thesis deals with double well potentials. We will study the behaviour of eigenfunctions of the Schrödinger operator $P(h) = -h^2\partial_x^2 + V(x)$ where the double well potential V is symmetric. Following Jona-Lasinio et al. [9], Helffer and Sjöstrand [3] and [4], and Simon [7], we will study the consequences of a small perturbation ΔV that breaks the symmetry of V.

Contents

1 Introduction

Two topics will be discussed in this thesis. In the first part, we will discuss semiclassical analysis as presented by Zworski [8]. We will consider certain classes of functions $a : \mathbb{R}^{2n} \to \mathbb{C}, (x, \xi) \mapsto a(x, \xi)$, and associate such functions with semiclassical pseudodifferential operators, i.e. pseudodifferential operators that are scaled with a small parameter $h > 0$. We will study the behaviour of such operators in the semiclassical limit $h \to 0$.

In the context of quantum mechanics, we interpret $\mathbb{R}^{2n}$ as the phase space. Then x is the position variable and ξ is the momentum variable, and a function $a : \mathbb{R}^{2n} \to \mathbb{C}$ is called a symbol. Then the corresponding operator $a^W(x, hD)$ is a quantum observable, and the semiclassical limit $h \to 0$ is actually the classical limit of quantum mechanics.

An important example is the total energy function $p(x, \xi) := |\xi|^2 + V(x)$, where $|\xi|^2$ is the kinetic energy and V is the potential. This symbol gives rise to the Schrödinger operator $P(h) := -h^2\Delta + V$. We will prove the Agmon-Lithner estimate and the Carleman inequality for eigenfunctions of this operator in the limit $h \to 0$.

We will need some preliminary definitions, which we will give in section 2. In section 3, we will give an overview of semiclassical Fourier analysis, which is just a rescaling of standard Fourier analysis by a parameter $h > 0$. The Fourier transformation will first be defined on the Schwartz space $\mathscr{S}(\mathbb{R}^n)$. We will then generalise the Fourier transformation to the dual space $\mathscr{S}'(\mathbb{R}^n)$.

Section 4 deals with semiclassical quantisation. We will again start with symbols in $\mathscr{S}(\mathbb{R}^{2n})$, which give rise to bounded operators $L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$. We will then discuss larger classes of symbols $S_\delta(m)$ where $0 \leq \delta \leq 1/2$ and m is a so-called order function. Such symbols give rise to operators $\mathscr{S}'(\mathbb{R}^n) \to \mathscr{S}'(\mathbb{R}^n)$. We will prove that symbols in $S = S_0(1)$ give rise to bounded operators $L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$.

In section 5, we will prove several important inequalities. We will first prove the Gårding inequality for symbols $a \in S$. Then we will prove the Agmon-Lither estimate and the Carleman estimate for eigenfunctions of $P(h)$.

In the second part, we will apply these results to a potential V that has multiple wells, following several papers from the 1980s. The main goal of this part is to provide a focused and detailed approach to the ideas presented by B. Helffer and J. Sjöstrand in [3] and [4] and by B. Simon in [7]. Two other important papers are Jona-Lasinio et al. [9] and Graffi et al. [10].

In section 6, we will consider the symmetric double-well potential, following Helffer [2]. The splitting of the lowest two eigenvalues of $P(h)$ is of order $\tilde{O}(e^{-\delta_0/h})$, and the eigenfunctions corresponding to these eigenvalues are symmetric. In section 7, we will consider a slightly perturbed potential $\tilde{V} = V + t\Delta V$ where $t \in [-1, 1]$. Surprisingly, even a very small perturbation has drastic consequences for the eigenfunctions. If ΔV is supported close to one of the wells, the eigenfunctions will be localised in just one of the wells, even if $t = e^{-\gamma/h}$ for some sufficiently small constant $\gamma > 0$. As a result, the perturbed eigenfunctions are not even approximately symmetric.

1.1 acknowledgment

I would like to thank my supervisor Klaas Landsman for his advice and patience.

2 Introduction to the Schrödinger equation

In this section, we will introduce the position and momentum operators, as well as the Schrödinger operator $P(h)$ and its eigenfunctions.

2.1 Wave functions

In classical physics, a particle's state is just its position x and its momentum $p := m\dot{x}$. These develop over time according to the differential equation $F = m\partial_t^2 x$, where $\partial_t := \frac{d}{dt}$. In quantum mechanics, a particle's position and momentum are not localised as points in phase-space. Instead, a particle's state is given by its so-called wave function $u : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}, (t, x) \mapsto u(t, x)$.

This wave function u is a probability amplitude in the sense that $|u(x)|^2 = \overline{u(x)}u(x)$ is a probability density function, i.e. the probability of finding the particle in $U \subseteq \mathbb{R}^n$ is given by $\|u\|_{L^2(U)}$. For this reason, we have $u \in L^2(\mathbb{R}^n)$ and $\|u\|_{L^2(\mathbb{R}^n)} = 1$. Moreover, wave functions solve the Schrödinger equation

$$i\hbar\partial_t u(t, x) = -\frac{\hbar^2}{2m}\Delta u(t, x) + V(x)u(t, x) \tag{2.1}$$

where $\hbar$ is the Planck constant, m the particle's mass, and the map $V : \mathbb{R}^n \to \mathbb{R}$ is the potential.

We will simplify this equation by setting $m = 1/2$ and replacing $\hbar$ with a dimensionless constant $h > 0$. Moreover, we will consider stationairy states, i.e. functions u such that $ih\partial_t u \equiv 0$.

Definition 2.1. *(Schrödinger operator) Let $h > 0$ and let $V : \mathbb{R}^n \to \mathbb{R}$ be a smooth function not depending on h, then the Schrödinger operator $P(h)$ is defined by*

$$P(h)u = -h^2\Delta u + Vu, \tag{2.2}$$

In subsections 2.3 and 2.4, we will define the appropriate domain of $P(h)$ as well as what it means for a function u to solve the time-independent Schrödinger equation $P(h)u = E(h)u$.

2.2 Position and momentum operators

We will now consider the position operator X_j and the momentum operator P_j, where $1 \le j \le n$. For any wave function $u \in L^2(\mathbb{R}^n)$, $\|u\| = 1$, the expectation values are $\langle u, X_j u\rangle$ and $\langle u, P_j u\rangle$. We will use the convention that

$$D_{x_j} := \frac{1}{i}\frac{\partial}{\partial x_j}.$$

Then

$$\begin{aligned}
\langle u, X_j u\rangle &= \mathbb{E}_u(X_j) = \int_{\mathbb{R}^n} dx\, \left[x_j |u(x)|^2\right] \\
&= \langle u, x_j u\rangle_{L^2}, \\
\langle u, P_j u\rangle &= \mathbb{E}_u(P_j) = \frac{1}{2}\partial_t \mathbb{E}_u(X_j) \\
&= \int_{\mathbb{R}^n} dx\, \left[\frac{1}{2}x_j\partial_t(\overline{u(x)}u(x))\right] = \int_{\mathbb{R}^n} dx\, \left[\frac{1}{2}x_j\left((\partial_t\overline{u(x)})u(x) + \overline{u(x)}(\partial_t u(x))\right)\right] \\
&= \int_{\mathbb{R}^n} dx\left[\frac{1}{2}x_j\left(\frac{1}{-ih}(-h^2\overline{\Delta u(x)} + V(x)\overline{u(x)})u(x) + \overline{u(x)}\frac{1}{ih}(-h^2\Delta u(x) + V(x)u(x))\right)\right] \\
&= \int_{\mathbb{R}^n} dx\, \left[\frac{h}{2i}x_j\left(\overline{\Delta u(x)}u(x) - \overline{u(x)}\Delta u(x)\right)\right] = \int_{\mathbb{R}^n} dx\, \left[\frac{h}{2}x_j iD\cdot\left(u(x)\overline{Du(x)} - \overline{u(x)}Du(x)\right)\right] \\
&= -\int_{\mathbb{R}^n} dx\, \left[\frac{h}{2}e_j\cdot\left(u(x)\overline{Du(x)} - \overline{u(x)}Du(x)\right)\right] = \int_{\mathbb{R}^n} dx\, \left[\overline{u(x)}hD_{x_j}u(x)\right] \\
&= \langle u, hD_{x_j}u\rangle_{L^2}.
\end{aligned}$$

Hence $X_j u = x_j u$ and $P_j u = hDu$. In order to avoid confusion, we will always denote the momentum operator by hD.

2.3 Sobolev spaces

We have seen that wave functions u are quadratically integrable, i.e. $u \in L^2(\mathbb{R}^n)$, and that they need to satisfy the Schrödinger equation (equation 2.1). However, most functions in $L^2(\mathbb{R}^n)$ are not differentiable. To overcome this problem, we will recall the notion of weak derivative and the Sobolev function space $H^k(\mathbb{R}^n)$.

Definition 2.2. *(Test functions) Let $U \subseteq \mathbb{R}^n$ be open, then a function $\varphi : U \to \mathbb{C}$ is called a test function if it is smooth and compactly supported. The space of such functions is denoted by $C_c^\infty(U)$.*

Note that test functions vanish at the boundary ∂U. This follows from the fact that they are supported on a compact subset of U and the fact that U is open.

Now let $\varphi \in C_c^\infty(U)$ and let $\alpha := (\alpha_1, \ldots, \alpha_n)$ be a multi-index (i.e. $\alpha \in \mathbb{N}^n$) such that $|\alpha| := \alpha_1 + \ldots + \alpha_n \leq k$. If we assume that $u \in C^k(U)$, then the partial derivative

$$D^\alpha u := \frac{1}{i^{|\alpha|}} \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_n}} u \tag{2.3}$$

exists, and we can obtain the equality

$$\int_U dx[u(x) D^\alpha \varphi(x)] = (-1)^{|\alpha|} \int_U dx[D^\alpha u(x) \varphi(x)]$$

by integrating by parts $|\alpha|$ times. In case $u \notin C^k(U)$, we will use this equation to define generalise $D^\alpha u$. Let v be some function. We want

$$\int_U dx[u(x) D^\alpha \varphi(x)] = (-1)^{|\alpha|} \int_U dx[v(x) \varphi(x)],$$

because then we can set $D^\alpha u := v$. Clearly, these integrals can only exist if the functions u and v are integrable on $\mathrm{Supp}(\varphi)$ for all $\varphi \in C_c^\infty(U)$. This motives the following two definitions.

Definition 2.3. *(Locally integrable functions) Let $U \subseteq \mathbb{R}^n$ be open and let $u : U \to \mathbb{C}$ be a function. Then u is called locally integrable if*

$$u|_V \in L^1(V)$$

for all open $V \subset\subset U$, i.e. for all open $V \subseteq U$ such that $\overline{V}$ is compact and $\overline{V} \subset U$. The set of locally integrable functions is denoted $L^1_{loc}(U)$.

Definition 2.4. *(Weak derivatives) Let $u, v \in L^1_{loc}(U)$ and let α be a multi-index, then $D^\alpha u := v$ is called the weak α^{th} partial derivative of u if*

$$\int_U dx[u(x) D^\alpha \varphi(x)] = (-1)^{|\alpha|} \int_U dx[v(x) \varphi(x)]$$

for all $\varphi \in C_c^\infty(U)$.

Lemma 2.5. *(Uniqueness of weak derivatives) Weak derivatives are unique up to sets of Lebesgue-measure zero.*

Proof. Let $u, v, v' \in L^1_{\text{loc}}(U)$ and let $\alpha := (\alpha_1, \ldots, \alpha_n)$ be a multi-index. Assume that v and v' are weak α^{th} partial derivatives of u. Then we have for all test functions $\varphi \in C_c^\infty(U)$ that

$$(-1)^{|\alpha|} \int_U dx[v(x) \varphi(x)] = \int_U dx[u(x) D^\alpha \varphi(x)] = (-1)^{|\alpha|} \int_U dx[v'(x) \varphi(x)].$$

But then we have

$$\int_U dx[(v(x) - v'(x)) \varphi(x)] = 0$$

for all $\varphi \in C_c^\infty(U)$, hence $v = v'$ almost everywhere. □

Of course, weak derivatives need not exist in general. We will consider spaces of square integrable functions that have weak derivatives up to some degree $k \in \mathbb{N}$.

Definition 2.6. *(Sobolev spaces) Let $U \in \mathbb{R}^n$ be open and let $k \in \mathbb{N}$, then the Sobolev space $H^k(U)$ consists of all functions $u \in L^2(U)$ have weak derivatives $D^\alpha u \in L^2(U)$ for all multi-indices α such that $|\alpha| \leq k$.*

We can define an inner product on $H^k(U)$ by

$$\langle u, v\rangle_{H^k(U)} := \sum_{|\alpha|\leq k} \langle D^\alpha u, D^\alpha v\rangle_{L^2(U)}, \tag{2.4}$$

making $H^k(U)$ into a Hilbert space.

2.4 Weak solutions

The definition of weak solutions u of $P(h)u = E(h)u$ is analogous to the definition of the weak derivative. Let u such that $P(h)u = E(h)u$ and let v be some function. Then

$$\begin{aligned}
0 &= \langle v, (P(h) - E(h))u\rangle \\
&= \int_{\mathbb{R}^n} dx \left[\overline{v(x)}\left(-h^2\Delta u(x) + V(x)u(x) - E(h)u(x)\right)\right] \\
&= -h^2 \sum_{j=1}^n \int_{\mathbb{R}^n} dx \left[\overline{v(x)}\partial_j^2 u(x)\right] + \int_{\mathbb{R}^n} dx \left[\overline{v(x)}(V(x) - E(h))u(x)\right] \\
&= h^2 \sum_{j=1}^n \int_{\mathbb{R}^n} dx \left[\overline{\partial_j v(x)}\partial_j u(x)\right] + \int_{\mathbb{R}^n} dx \left[\overline{v(x)}(V(x) - E(h))u(x)\right] \\
&= \langle v, (V - E(h))u\rangle + \sum_{j=1}^n \langle hD_j v, hD_j u\rangle.
\end{aligned}$$

Definition 2.7. *(Weak solutions of the Schrödinger equation) A function $u \in H^1(\mathbb{R}^n)$ possibly depending on h is called a weak solution of $P(h)u = E(h)u$ if*

$$\langle v, (V - E)u\rangle + \sum_{j=1}^n \langle hD_j v, hD_j u\rangle = 0 \tag{2.5}$$

for all $v \in C_c^\infty(\mathbb{R}^n)$. A function $u \in H^1(\mathbb{R}^n)$ is called a solution to the Schrödinger equation if it is a weak solution of $P(h)u = E(h)u$ and $\|u\|_{L^2(\mathbb{R}^n)} = 1$.

Since we mostly deal with the momentum operator hD instead of the differential operator D, it makes sense to scale the Sobolev norm accordingly.

Definition 2.8. *(Semiclassical Sobolev norm) Let $U \subseteq \mathbb{R}^n$ be open. The semiclassical Sobolev norm on the space $H^k(U)$ is given by*

$$\|u\|_{H_h^k(U)} := \left(\sum_{|\alpha|\leq k} \|hD^\alpha u\|^2_{L^2(U)}\right)^{1/2}. \tag{2.6}$$

3 Semiclassical Fourier analysis

In this section, we will discuss semiclassical Fourier theory. The semiclassical Fourier transform $\mathscr{F}_h$ is a rescaling of the standard Fourier transform using the parameter $h > 0$. Then $\mathscr{F}_h$ maps $\varphi(x)$ into $\hat{\varphi}_h(\xi)$ such that $(hD)^\alpha\varphi \mapsto \xi^\alpha\hat{\varphi}_h$ and $(-x)^\alpha\varphi \mapsto (hD)^\alpha\hat{\varphi}_h$.

3.1 Schwartz space $\mathscr{S}(\mathbb{R}^n)$

Our goal is to define the semiclassical Fourier transform on a large class of functions, but we will start with just the so-called Schwartz functions. Schwartz functions behave very nicely in the sense that all their derivatives decrease rapidly as $|x| \to \infty$, as does the function itself. An example of such a function is the Gaussian function $\varphi(x) := e^{-\pi|x|^2}$.

Definition 3.1. *(Schwartz space) The Schwartz space $\mathscr{S}(\mathbb{R}^n)$ consists of all functions $\varphi \in C^\infty(\mathbb{R}^n)$ such that*

$$\sup_{x\in\mathbb{R}^n} |x^\alpha\partial^\beta\varphi(x)| < \infty$$

for all multi-indices α, β.

Note that $\|\varphi\|_{\alpha,\beta} := \sup_{x\in\mathbb{R}^n} |x^\alpha\partial^\beta\varphi(x)|$ is a seminorm on $\mathscr{S}(\mathbb{R}^n)$ for each pair of multi-indices α, β. This collection of seminorms defines a topology on $\mathscr{S}$ as follows. Consider

$$V(\alpha, \beta, k) := \{\varphi \in \mathscr{S}(\mathbb{R}^n) \mid \|\varphi\|_{\alpha,\beta} < \frac{1}{k}\}.$$

The collection of finite intersections of such sets is a convex, balanced local base of a topology in $\mathscr{S}(\mathbb{R}^n)$ turning it into a locally convex space such that all seminorms are continuous.

A subset $U \subset \mathscr{S}(\mathbb{R}^n)$ is bounded if and only if $\{\|\varphi\|_{\alpha,\beta} \mid \varphi \in U\}$ is bounded for all multi-indices α, β. It should be noted that all $\|\cdot\|_{\alpha,\beta}$ are actually norms, and that the spaces $\mathscr{S}(\mathbb{R}^n)$ with this norm is a Fréchet space.

It is easy to see that $C_c^\infty(\mathbb{R}^n) \subset \mathscr{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$. Recall that $C_c^\infty(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$, then it follows trivially that $\mathscr{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ in the L^2-norm.

Definition 3.2. *(Semiclassical Fourier transform) Let $\varphi \in \mathscr{S}$, then its semiclassical Fourier transform $\hat{\varphi}_h$ is defined by*

$$\hat{\varphi}_h(\xi) := \mathscr{F}_h(\varphi)(\xi) := \int_{\mathbb{R}^n} dx \left[\varphi(x)e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \tag{3.1}$$

where $\xi \in \mathbb{R}^n$.

Remark 3.3. *In case $h = 1$, we also write $\mathscr{F} := \mathscr{F}_1$ and $\hat{\varphi} := \hat{\varphi}_1$, which is the standard Fourier transform. Note that some authors define the Fourier transform with a normalisation factor $1/(2\pi h)^{n/2}$.*

Proposition 3.4. *(Properties of the semiclassical Fourier transform) The semiclassical Fourier transform $\mathscr{F}_h : \mathscr{S} \to \mathscr{S}$ is an isomorphism, whose inverse is given by*

$$\varphi(x) = \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\hat{\varphi}_h(\xi)e^{\frac{i}{h}\langle x,\xi\rangle}\right]$$

for all $x \in \mathbb{R}^n$. Furthermore, we have the following equalities:

(i) $\mathscr{F}_h((hD_x)^\alpha\varphi) = \xi^\alpha\mathscr{F}_h(\varphi)$,

(ii) $\mathscr{F}_h((-x)^\alpha\varphi) = (hD_\xi)^\alpha(\mathscr{F}_h(\varphi))$.

Proof. We will only show that equalities (i) and (ii) hold. The other statements are well-known facts from standard Fourier theory. Let $\xi \in \mathbb{R}^n$, then we have

$$\begin{aligned}
\mathscr{F}_h((hD_x)^\alpha\varphi)(\xi) &= \int_{\mathbb{R}^n} dx \left[(hD_x)^\alpha \varphi(x) e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= (-1)^{|\alpha|}\int_{\mathbb{R}^n} dx \left[\varphi(x)(hD_x)^\alpha e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= (-1)^{|\alpha|}\int_{\mathbb{R}^n} dx \left[\varphi(x)\left(\frac{h}{i}\right)^\alpha \left(-\frac{i}{h}\xi\right)^\alpha e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= \xi^\alpha \int_{\mathbb{R}^n} dx \left[\varphi(x) e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= \xi^\alpha \mathscr{F}_h(\varphi)(\xi), \\
(hD_\xi)^\alpha(\mathscr{F}_h(\varphi))(\xi) &= (hD_\xi)^\alpha \int_{\mathbb{R}^n} dx \left[\varphi(x) e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= \int_{\mathbb{R}^n} dx \left[\varphi(x)(hD_\xi)^\alpha e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= \int_{\mathbb{R}^n} dx \left[\varphi(x)(-x)^\alpha e^{-\frac{i}{h}\langle x,\xi\rangle}\right] \\
&= \mathscr{F}_h((-x)^\alpha\varphi)(\xi).
\end{aligned}$$

□

Lemma 3.5. *(More properties) Let $\varphi, \psi \in \mathscr{S}$, then we have*

$$\int_{\mathbb{R}^n} dx\,[\mathscr{F}_h(\varphi)(x)\psi(x)] = \int_{\mathbb{R}^n} dx\,[\varphi(x)\mathscr{F}_h(\psi)(x)] \tag{3.2}$$

and

$$\int_{\mathbb{R}^n} dx \left[\overline{\varphi(x)}\psi(x)\right] = \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} dx \left[\overline{\mathscr{F}_h(\varphi)(x)}\mathscr{F}_h(\psi)(x)\right]. \tag{3.3}$$

Proof.

$$\begin{aligned}
\int_{\mathbb{R}^n} dx\,[\mathscr{F}_h(\varphi)(x)\psi(x)] &= \int_{\mathbb{R}^n} dx \left[\int_{\mathbb{R}^n} dy \left[\varphi(y) e^{-\frac{i}{h}\langle y,x\rangle}\right]\psi(x)\right] \\
&= \int_{\mathbb{R}^n} dy \left[\int_{\mathbb{R}^n} dx \left[\psi(x) e^{-\frac{i}{h}\langle x,y\rangle}\right]\varphi(y)\right] \\
&= \int_{\mathbb{R}^n} dx\,[\varphi(x)\mathscr{F}_h(\psi)(x)]
\end{aligned}$$

This proves equation (3.2). Now we can substitute φ with $\overline{\mathscr{F}_h(\varphi)}$ to obtain

$$\int_{\mathbb{R}^n} dx \left[\overline{\mathscr{F}_h(\varphi)(x)}\mathscr{F}_h(\psi)(x)\right] = \int_{\mathbb{R}^n} dx \left[\mathscr{F}_h(\overline{\mathscr{F}_h(\varphi)})(x)\psi(x)\right].$$

Note that $\overline{\mathscr{F}_h(\varphi)(\xi)} = \int_{\mathbb{R}^n} dy \left[\overline{\varphi(x)} e^{\frac{i}{h}\langle y,\xi\rangle}\right] = (2\pi h)^n \mathscr{F}_h^{-1}(\overline{\varphi})(\xi)$, so

$$\mathscr{F}_h(\overline{\mathscr{F}_h(\varphi)})(x) = (2\pi h)^n \overline{\varphi(x)}.$$

□

Hence $\|\hat{\varphi}_h\| = (2\pi h)^{n/2}\|\varphi\|$. We will now prove a few norm estimates that will prove useful later. The notation $\langle x\rangle := (1+|x|^2)^{1/2}$ will be convenient. Note that $\int_{\mathbb{R}^n} dx[\langle x\rangle^{-(n+1)}] < \infty$ and there is a constant $C > 0$ such that $\langle x\rangle^k \le C \max_{|\alpha|\le k}|x^\alpha|$ for all $x \in \mathbb{R}^n$, $k \in \mathbb{N}$.

Lemma 3.6. *(norm estimates) Let $u \in \mathscr{S}$ and $h > 0$, then there is some constant $C > 0$ such that*

$$\|\hat{u}_h\|_{L^\infty} \le \|u\|_{L^1} \tag{3.4}$$

$$\|u\|_{L^\infty} \le \frac{1}{(2\pi h)^n}\|\hat{u}_h\|_{L^1} \tag{3.5}$$

$$\|\hat{u}_h\|_{L^1} \le C \max_{|\alpha|\le n+1}\|\partial^\alpha u\|_{L^1} \tag{3.6}$$

Proof.

$$
\begin{aligned}
\|\hat{u}_h\|_{L^\infty} &= \sup_{\xi\in\mathbb{R}^n} |\hat{u}_h(\xi)| = \sup_{\xi\in\mathbb{R}^n} \left| \int_{\mathbb{R}^n} dx \left[u(x) e^{\frac{i}{h}\langle x,\xi\rangle} \right] \right| \\
&\le \sup_{\xi\in\mathbb{R}^n} \int_{\mathbb{R}^n} dx \left| u(x) e^{\frac{i}{h}\langle x,\xi\rangle} \right| = \sup_{\xi\in\mathbb{R}^n} \int_{\mathbb{R}^n} dx |u(x)| \\
&= \|u\|_{L^1} \\
\|u\|_{L^\infty} &= \sup_{x\in\mathbb{R}^n} |u(x)| = \sup_{x\in\mathbb{R}^n} \left| \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\hat{u}_h(\xi) e^{\frac{i}{h}\langle x,\xi\rangle} \right] \right| \\
&\le \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left| \hat{u}_h(\xi) e^{\frac{i}{h}\langle x,\xi\rangle} \right| \\
&= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi |\hat{u}_h(\xi)| = \frac{1}{(2\pi h)^n} \|\hat{u}_h\|_{L^1} \\
\|\hat{u}_h\|_{L^1} &= \int_{\mathbb{R}^n} d\xi |\hat{u}_h(\xi)| = \int_{\mathbb{R}^n} d\xi \left[|\hat{u}_h(\xi)| \langle\xi\rangle^{n+1} \langle\xi\rangle^{-(n+1)} \right] \\
&\le C \int_{\mathbb{R}^n} d\xi \left[\langle\xi\rangle^{-(n+1)} \max_{|\alpha|\le n+1} |\hat{u}_h(\xi)\xi^\alpha| \right] \\
&\le C \max_{|\alpha|\le n+1} \|\hat{u}_h \xi^\alpha\|_{L^\infty} \int_{\mathbb{R}^n} d\xi \left[\langle\xi\rangle^{-(n+1)} \right] \\
&\le C \max_{|\alpha|\le n+1} \|\hat{u}_h \xi^\alpha\|_{L^\infty} \le C \max_{|\alpha|\le n+1} \|\partial^\alpha u\|_{L^1}
\end{aligned}
$$

□

3.2 Tempered distributions $\mathscr{S}'(\mathbb{R}^n)$

The Schwartz space is very small class of functions, so our goal is to extend the Fourier transform to a wider class of functions. Let $u : \mathbb{R}^n \to \mathbb{C}$ be a quadratically integrable function. Then we can define a continuous linear map $u : \mathscr{S} \to \mathbb{C}$ by $u(\varphi) := \int_{\mathbb{R}^n} dx\, [u(x)\varphi(x)]$. This will serve as motivation for the following definition.

Definition 3.7. *(Tempered distributions) The set*

$$\mathscr{S}'(\mathbb{R}^n) := \{u : \mathscr{S} \to \mathbb{C} \mid u \text{ is linear and continuous } \} \tag{3.7}$$

is the dual space of $\mathscr{S}(\mathbb{R}^n)$ and maps $u \in \mathscr{S}'$ are called tempered distributions.
A sequence $\{u_j\}_{j\in\mathbb{N}} \subset \mathscr{S}'$ is said to converge in $\mathscr{S}'$ if there is a map $u \in \mathscr{S}'$ such that $\{u_j(\varphi)\}_{j\in\mathbb{N}} \subset \mathbb{C}$ converges to $u(\varphi)$ for all $\varphi \in \mathscr{S}$.

For $u \in \mathscr{S}'$, we will sometimes write

$$\int_{\mathbb{R}^n} dx\, [u(x)\varphi(x)] := u(\varphi)$$

even though such a locally integrable function $u : \mathbb{R}^n \to \mathbb{C}$ does not exist in general.

Definition 3.8. *(More on tempered distributions) Let $u \in \mathscr{S}'$ and $\varphi \in \mathscr{S}$. Let α be a multi-index and let $x \in \mathbb{R}^n$, then we define:*

(i) $D^\alpha u(\varphi) := (-1)^{|\alpha|} u(D^\alpha \varphi)$*, in the same spirit as the weak derivative. Note that $D^\alpha\varphi$ and hence $D^\alpha u$ is guaranteed to exist.*

(ii) $(x^\alpha u)(\varphi) := u(x^\alpha \varphi)$

(iii) We take equation (3.2) as a definition for the semiclassical Fourier transform on tempered distributions, i.e. $(\mathscr{F}_h u)(\varphi) := u(\mathscr{F}_h \varphi)$.

Example 3.9. *(Dirac delta function) Let $x_0 \in \mathbb{R}^n$, then we define the Dirac delta function δ_{x_0} at x_0 by $\delta_{x_0}(\varphi) := \varphi(x_0)$ for all $\varphi \in \mathscr{S}$. One can think of the Dirac delta function as a function that is infinite* *at x_0 and zero everywhere else, such that its integral is $\int_{\mathbb{R}^n} dx[\delta_{x_0}(x)] = 1$. Then we have for any $\varphi \in \mathscr{S}$ that $\int_{\mathbb{R}^n} dx[\delta_{x_0}(x)\varphi(x)] = \varphi(x_0)$.*

We can calculate its Fourier transform by

$$(\mathscr{F}_h \delta_{x_0})(\varphi) := \delta_{x_0}(\mathscr{F}_h \varphi) = \mathscr{F}_h \varphi(x_0) = \int_{\mathbb{R}^n} dx[\varphi(x) e^{-\frac{i}{h}\langle x, x_0 \rangle}].$$

In other words, $\mathscr{F}_h \delta_{x_0}(x) := e^{-\frac{i}{h}\langle x, x_0 \rangle}$. In particular, $\mathscr{F}_h(\delta_0) \equiv 1$.

Many of the properties of $\mathscr{F}_h : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$ hold more generally.

Remark 3.10. *(Semiclassical Fourier transform on L^2) Let $u \in L^2(\mathbb{R}^n)$, then we can interpret u as a tempered distribution defined by*

$$\varphi \mapsto \int_{\mathbb{R}^n} dx\,[u(x)\varphi(x)]$$

where $\varphi \in \mathscr{S}$. Then we have for the semiclassical Fourier transform $\hat{u}_h$ of $u \in L^2$ that

$$\begin{aligned}\int_{\mathbb{R}^n} d\xi\,[\hat{u}_h(\xi)\varphi(\xi)] &:= \int_{\mathbb{R}^n} dx\,[u(x)\hat{\varphi}_h(x)] = \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} d\xi \left[u(x)\varphi(\xi) e^{-\frac{i}{h}\langle x, \xi \rangle}\right] \\ &= \int_{\mathbb{R}^n} d\xi \left[\int_{\mathbb{R}^n} dx \left(u(x) e^{-\frac{i}{h}\langle x, \xi \rangle}\right) \varphi(\xi)\right]\end{aligned}$$

for all $\varphi \in \mathscr{S}$. So equation (3.1) is still valid for L^2-functions. The same is true for the inverse semiclassical Fourier transform. As a result, lemma 3.5 holds for L^2-functions as well.

Proposition 3.11. *(Properties of the semiclassical Fourier transform on tempered distributions) Let $u \in \mathscr{S}', x, \xi \in \mathbb{R}^n$, and let α be a multi-index. Then we have*

(i) $\mathscr{F}_h((hD_x)^\alpha u) = \xi^\alpha \mathscr{F}_h(u)$, and

(ii) $\mathscr{F}_h((-x)^\alpha u) = (hD_\xi)^\alpha \mathscr{F}_h(u)$.

Proof. For all $\varphi \in \mathscr{S}$, we have

$$\begin{aligned}\mathscr{F}_h((hD)^\alpha u) &= (hD)^\alpha u(\mathscr{F}_h(\varphi)) = (-1)^{|\alpha|} u((hD)^\alpha \mathscr{F}_h(\varphi)) \\ &= (-1)^{|\alpha|} u(\mathscr{F}_h((-x)^\alpha \varphi))) = \mathscr{F}_h(u)(\xi^\alpha \varphi) \\ &= \xi^\alpha \mathscr{F}_h(u)(\varphi) \\ \mathscr{F}_h((-x)^\alpha u)(\varphi) &= (-\xi)^\alpha u(\mathscr{F}_h(\varphi)) = u((-\xi)^\alpha \mathscr{F}_h(\varphi)) \\ &= (-1)^\alpha u(\mathscr{F}_h((hD)^\alpha \varphi)) = (-1)^\alpha \mathscr{F}_h(u)((hD)^\alpha \varphi) \\ &= (hD)^\alpha \mathscr{F}_h(u)(\varphi)\end{aligned}$$

□

3.3 Uncertainty principle

In this subsection, we will prove Heisenberg's uncertainty principle. Let $u \in \mathscr{S}(\mathbb{R}^n)$ such that $\|u\| = 1$ and let $1 \leq j \leq N$. Consider the standard deviation of position σ_{x_j} and the standard deviation of momentum σ_{hD_j}. Note that

$$\begin{aligned}\sigma_{x_j}^2 &= \langle u, x_j^2 u \rangle - \langle u, x_j u \rangle^2, \\ \sigma_{hD_j}^2 &= \langle u, (hD_j)^2 u \rangle - \langle u, hD_j u \rangle^2.\end{aligned}$$

Then Heisenberg's uncertainty principle states that $\sigma_{x_j}\sigma_{hD_j} \geq h/2$. We interpret that the position and the momentum of a physical state cannot be localised simultaneously.

The relation between a wave function $u(x)$ and its semiclassical Fourier transform $\hat{u}_h(\xi)$ is characterised by equation (3.3), i.e. for $u \in \mathscr{S}(\mathbb{R}^n)$, the expectation values for the position and momentum operators in direction $1 \leq j \leq n$ are given by

$$\begin{aligned}\langle u, x_j u\rangle &= \int_{\mathbb{R}^n} dx \left[\overline{u(x)} x_j u(x)\right] = \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{\mathscr{F}_h(u)(\xi)} \mathscr{F}_h(x_j u)(\xi)\right] \\ &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{\hat{u}_h(\xi)}(-hD_j)\hat{u}_h(\xi)\right] = \frac{1}{(2\pi h)^n} \langle \hat{u}_h, -hD_j \hat{u}_h\rangle, \\ \langle u, hD_j u\rangle &= \int_{\mathbb{R}^n} dx \left[\overline{u(x)} hD_j u(x)\right] = \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{\mathscr{F}_h(u)(\xi)} \mathscr{F}_h(hD_j u)(\xi)\right] \\ &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{\hat{u}_h(\xi)} \xi_j \hat{u}_h(\xi)\right] = \frac{1}{(2\pi h)^n} \langle \hat{u}_h, \xi_j \hat{u}_h\rangle.\end{aligned}$$

For this reason, $u(x)$ is said to be the wave function in position coordinates, and $\hat{u}_h(\xi)$ the wave function in momentum coordinates.

Lemma 3.12. *(Shifting the position coordinates) Let $u \in \mathscr{S}(\mathbb{R}^n)$ such that $\|u\|_{L^2(\mathbb{R}^n)} = 1$ and let $a \in \mathbb{R}^n$, then we can shift the coordinates by setting $x \rightsquigarrow y := x - a$ and $v(y) := u(y + a)$. The shifted wave function v satisfies $\langle v, yv\rangle = \langle u, xu\rangle - a$ and $\langle v, hDv\rangle = \langle u, hDu\rangle$.*

Proof. This is a fairly straightforward computation. Let $1 \leq j \leq n$, then

$$\begin{aligned}\langle v, y_j v\rangle &= \int_{\mathbb{R}^n} dy \left[\overline{v(y)} y_j v(y)\right] = \int_{\mathbb{R}^n} dy \left[\overline{u(y+a)} y_j u(y+a)\right] \\ &= \int_{\mathbb{R}^n} dx \left[\overline{u(x)} (x_j - a_j) u(x)\right] = \langle u, x_j u\rangle - a_j, \\ \hat{v}_h(\xi) &= \int_{\mathbb{R}^n} dy \left[v(y) e^{-\frac{i}{h}\langle y, \xi\rangle}\right] = \int_{\mathbb{R}^n} dy \left[u(y+a) e^{-\frac{i}{h}\langle y, \xi\rangle}\right] \\ &= \int_{\mathbb{R}^n} dx \left[u(x) e^{-\frac{i}{h}\langle x - a, \xi\rangle}\right] = e^{\frac{i}{h}\langle a, \xi\rangle} \hat{u}_h(\xi), \\ \langle \hat{v}_h, \xi_j \hat{v}_h\rangle &= \int_{\mathbb{R}^n} d\xi \left[\overline{\hat{v}_h(\xi)} \xi_j \hat{v}_h(\xi)\right] = \int_{\mathbb{R}^n} d\xi \left[\overline{e^{\frac{i}{h}\langle a, \xi\rangle} \hat{u}_h(\xi)} \xi_j e^{\frac{i}{h}\langle a, \xi\rangle} \hat{u}_h(\xi)\right] \\ &= \int_{\mathbb{R}^n} d\xi \left[\overline{\hat{u}_h(\xi)} \xi_j \hat{u}_h(\xi)\right] = \langle \hat{u}_h, \xi_j \hat{u}_h\rangle.\end{aligned}$$

□

Lemma 3.13. *(Shifting the momentum coordinates) Let $u \in \mathscr{S}(\mathbb{R}^n)$ such that $\|u\|_{L^2(\mathbb{R}^n)}$ and let $b \in \mathbb{R}^n$, then we can shift the coordinates by setting $\xi \rightsquigarrow \eta := \xi - b$ and $\hat{v}_h(\eta) := \hat{u}_h(\eta + b)$. The shifted wave function v satisfies $\langle v, xv\rangle = \langle u, xu\rangle$ and $\langle v, hDv\rangle = \langle u, hDu\rangle - b$.*

Proof. This is analogous to the previous lemma. □

Corollary 3.14. *By setting $a := \langle u, xu\rangle$ and $b := \langle u, hDu\rangle$, we obtain a shifted wave function v such that $\langle v, xv\rangle = \langle v, hDv\rangle = 0$. So for any $u \in \mathscr{S}(\mathbb{R}^n)$ such that $\|u\|_{L^2(\mathbb{R}^n)}$, we can assume without loss of generality that*

$$\begin{aligned}\sigma_{x_j}^2 &= \langle u, x_j^2 u\rangle = \|x_j u\|^2, \\ \sigma_{hD_j}^2 &= \langle u, (hD_j)^2 u\rangle = \|hD_j u\|^2.\end{aligned}$$

From now on, we will write $\|x_j u\|$ and $\|hD_j u\| = (2\pi h)^{-n/2}\|\xi_j \hat{u}_h\|$ instead of σ_{x_j} and σ_{hD_j}. Only one more lemma is needed before the uncertainty principle can be proved.

Lemma 3.15. *(Commutation relation of position and momentum) The commutation relation of the position and momentum operators x_j and hD_j as operators $\mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$ is given by*

$$[x_j, hD_j] := x_j hD_j - hD_j x_j = ih.$$

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$. Then we can simply compute that

$$[x_j, hD_j]u = x_j hD_j u - hD_j(x_j u) = \frac{h}{i}(x_j \partial_{x_j} u - \partial_{x_j}(x_j u)) = -\frac{h}{i} u = ihu.$$

□

Proposition 3.16. *(Heisenberg uncertainty principle) Let $u \in \mathscr{S}(\mathbb{R}^n)$, then*

$$\|x_j u\| \|\xi_j \hat{u}_h\| \geq \frac{h}{2} \|u\| \|\hat{u}_h\|. \tag{3.8}$$

In particular, if $\|u\|_{L^2(\mathbb{R}^n)} = 1$, then

$$\|x_j u\| \|hD_j u\| \geq \frac{h}{2}. \tag{3.9}$$

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$. Using the Cauchy-Schwarz inequality and the previous lemma we obtain

$$\begin{aligned}
\|x_j u\| \|hD_j u\| &\geq |\langle hD_j u, x_j u\rangle| \geq |\Im \langle hD_j u, x_j u\rangle| \\
&= \frac{1}{2} |\langle hD_j u, x_j u\rangle - \langle x_j u, hD_j u\rangle| \\
&= \frac{1}{2} |\langle (x_j hD_j - hD_j x)u, u\rangle| \\
&= \frac{1}{2} |\langle [x_j, hD_j]u, u\rangle| = \frac{h}{2} \|u\|^2,
\end{aligned}$$

hence

$$\|x_h u\| \|\xi_j \hat{u}_h\| = \|x_j u\| (2\pi h)^{n/2} \|hD_j u\| \geq \frac{h}{2} (2\pi h)^{n/2} \|u\|^2 = \frac{h}{2} \|u\| \|\hat{u}_h\|.$$

□

4 Semiclassical quantisation

In classical mechanics, the state of a system is completely determined by the position and momentum variables, and all dynamical quantities are a function of said variables. In the context of semiclassical quantisation, such a function is called a symbol. Examples are: the kinetic energy $T := \xi^2$ or the angular momentum $L := x \times \xi$ (where $\times$ is the outer product on $\mathbb{R}^3$).

In quantum mechanics, the operators associated with the position and momentum are x and hD, respectively. This raises the question what operators are associated with the other symbols. In this section, we will discuss this for various classes of symbols.

Definition 4.1. *(Symbols) A function $a : \mathbb{R}^{2n} \to \mathbb{R}, (x,\xi) \mapsto a(x,\xi)$ is called a symbol.*

Since x and hD do not commute, we can immediately see that there is no canonical way to quantise symbols that are linear in both arguments, such as $a(x,\xi) := \langle x, \xi\rangle$. We could pick any linear combination

$$a(x,\xi) = t\langle x, \xi\rangle + (1-t)\langle \xi, x\rangle.$$

This motivates the following definition.

Definition 4.2. *(Semiclassical quantisation) Let $t \in [0,1]$ and let $a(x,\xi)$ be a symbol, then the semiclassical pseudodifferential operator $Op_t(a)$ is defined by*

$$Op_t(a)u(x) := \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[a(tx + (1-t)y, \xi)u(y)e^{\frac{i}{h}\langle x-y,\xi\rangle}\right]. \tag{4.1}$$

In particular, we will be interested in the standard quantisation $a(x,hD) := Op_1(a)$ and the Weyl quantisation $a^W(x,hD) := Op_{\frac{1}{2}}(a)$.

Remark 4.3. *In subsections 4.1, we will show that $Op_t(a) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is indeed well-defined for symbols $a \in \mathscr{S}(\mathbb{R}^{2n})$. In subsection 4.3, we will show that $Op_t(a) : \mathscr{S}'(\mathbb{R}^n) \to \mathscr{S}'(\mathbb{R}^n)$ is well-defind for symbols $a \in S_\delta(m)$.*

The Weyl quantisation is the most important quantisation formula because it gives rise to a self-adjoint operator if the symbol a is real-valued. The standard quantisation is important because

$$\begin{aligned} a(x,hD)u(x) &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[a(x,\xi)u(y)e^{\frac{i}{h}\langle x-y,\xi\rangle}\right] \\ &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[a(x,\xi)\mathscr{F}_h u(\xi)e^{\frac{i}{h}\langle x,\xi\rangle}\right] \\ &= \mathscr{F}_h^{-1}(a(x,\cdot)\mathscr{F}_h u(\cdot))(x), \end{aligned}$$

for $a \in \mathscr{S}(\mathbb{R}^{2n})$ and $u \in \mathscr{S}(\mathbb{R}^n)$. This makes that standard quantisation easier to compute. The other Op_t are useful because they allow us to transfer computations from the standard quantisation to the Weyl quantisation, as we will see in the proof of lemma 4.38.

4.1 Semiclassical quantisation for $a \in \mathscr{S}(\mathbb{R}^{2n})$

The following defintion gives a very convenient way to abbreviate the formula for $Op_t(a)$.

Definition 4.4. *(Kernel of Op_t) Let $t \in [0,1]$, then we define the kernel K_t of Op_t by*

$$\begin{aligned} K_t(x,y) &:= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[a(tx + (1-t)y, \xi)e^{\frac{i}{h}\langle x-y,\xi\rangle}\right] \\ &= \mathscr{F}_h^{-1}(a(tx + (1-t)y, \cdot))(x-y). \end{aligned}$$

Note that $Op_t(a)u(x) = \int_{\mathbb{R}^n} dy\, [K_t(x,y)u(y)]$.

Now assume that $a \in \mathscr{S}(\mathbb{R}^{2n})$. Since $\mathscr{F}_h^{-1} : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$, we also have $K_t(x,\cdot) \in \mathscr{S}(\mathbb{R}^n)$. So for $u \in \mathscr{S}'(\mathbb{R}^n)$ we can define $Op_t(a)u \in \mathscr{S}(\mathbb{R}^n)$ by $Op_t(a)u(x) := u(K_t(x,\cdot))$.

Lemma 4.5. *Let $a \in \mathscr{S}(\mathbb{R}^{2n})$ be a symbol, $t \in [0,1]$, then $Op_t(a) : \mathscr{S}' \to \mathscr{S}$ is continuous.*

Proof. Consider a sequence $u_j \to u$ converging in $\mathscr{S}'(\mathbb{R}^n)$ and let α, β be multi-indices. Then

$$x^\alpha \partial^\beta (u(K_t(x,\cdot)) - u_j(K_t(x,\cdot))) = u(x^\alpha \partial^\beta K_t(x,\cdot)) - u_j(x^\alpha \partial^\beta K_t(x,\cdot)) \to 0,$$

hence $Op_t(a)u_j \to Op_t(a)u$ in $\mathscr{S}(\mathbb{R}^n)$ and $Op_t(a)$ is indeed continuous. □

Proposition 4.6. *Let $a \in \mathscr{S}(\mathbb{R}^{2n})$ and let $h > 0$, then the operator*

$$a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$$

is bounded uniformly in h, i.e. there is some constant $C > 0$ not depending on h such that we have $\|a^W(x,hD)u\| \leq C\|u\|$ for all $u \in L^2(\mathbb{R}^n)$.

Proof. We have $a \in \mathscr{S}(\mathbb{R}^{2n})$, and so $K_{1/2} \in \mathscr{S}(\mathbb{R}^{2n})$. Define the two constants

$$\begin{aligned} C_1 &:= \sup_{x\in\mathbb{R}^n} \int_{\mathbb{R}^n} dy \left[|K_{1/2}(x,y)|\right] < \infty, \\ C_2 &:= \sup_{y\in\mathbb{R}^n} \int_{\mathbb{R}^n} dx \left[|K_{1/2}(x,y)|\right] < \infty, \end{aligned}$$

then the L^2-norm of $a^W(x,hD)u$ is

$$\begin{aligned} \|a^W(x,hD)u\|^2 &= \langle a^W(x,hD)u, a^W(x,hD)u\rangle \\ &\leq \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} dy \int_{\mathbb{R}^n} dz \left[|K_{1/2}(x,y)||u(y)||K_{1/2}(x,z)||u(z)|\right] \\ &\leq \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} dy \int_{\mathbb{R}^n} dz \left[|K_{1/2}(x,y)||K_{1/2}(x,z)|\frac{1}{2}\left(|u(y)|^2 + |u(z)|^2\right)\right] \\ &= \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} dy \int_{\mathbb{R}^n} dz \left[|K_{1/2}(x,y)||K_{1/2}(x,z)||u(y)|^2\right] \\ &\leq C_1 C_2 \int_{\mathbb{R}^n} dy \left[|u(y)|^2\right] = C_1 C_2 \|u\|^2 \end{aligned}$$

□

Theorem 4.7. *Let $a \in \mathscr{S}(\mathbb{R}^{2n})$, then the operator $a^W(x,hD) : L^2 \to L^2$ is compact.*

Proof. Recall the definition of a compact operator (see C.1). The operator $a^W(x,hD)$ is compact if for any bounded sequence $\{u_k\}_{k\in\mathbb{N}} \subset L^2(\mathbb{R}^n)$, the sequence $\{a^W(x,hD)u_k\}_{k\in\mathbb{N}} \subset L^2(\mathbb{R}^{2n})$ has some converging subsequence.

Let $\{u_k\}_{k\in\mathbb{N}} \subset L^2(\mathbb{R}^n)$ be a bounded sequence and let $k, l \in \mathbb{N}$. We want to find a subsequence $\{u'_k\}$ of $\{u_k\}$ such that the sequence $\{a^W(x,hD)u'_k\}$ converges. Let $N \in \mathbb{N}$ be some fixed constant (we will later choose $N > n/2$), then we have for some sufficiently large constant $C > 0$ that

$$\begin{aligned} &\|a^W(x,hD)u_k - a^W(x,hD)u_l\|_{L^2} \\ &\quad = \int_{\mathbb{R}^n} dx \left[|a^W(x,hD)u_k(x) - a^W(x,hD)u_l|^2\right] \\ &\quad = \int_{\mathbb{R}^n} dx \left[\langle x\rangle^{-2N} |\langle x\rangle^N (a^W(x,hD)u_k(x) - a^W(x,hD)u_l(x))|^2\right] \\ &\quad \leq C\|\langle x\rangle^N (a^W(x,hD)u_k - a^W(x,hD)u_l)\|_{L^\infty}. \end{aligned}$$

So it suffices to show that the sequence $\{\langle x\rangle^N a^W(x,hD)u'_k\}$ converges in the sup-norm. We will first construct a candidate subsequence $\{u'_k\}$ and then prove that $\langle x\rangle^N a^W(x,hD)u'_k$ indeed converges uniformly.

For any $x \in \mathbb{R}^n$, the sequence $\{\langle x\rangle^N a^W(x,hD)u_k(x)\}_{k\in\mathbb{N}} \subset \mathbb{C}$ is bounded and therefore admits a converging subsequence. Consider some countable dense subset of $\mathbb{R}^n$, such as $\mathbb{Q}^n$. Enumerate these s.t. $\mathbb{Q}^n = \bigcup_{p\in\mathbb{N}}\{q_p\}$. We inductively define subsequences $\{u_k^{(j)}\}_{k\in\mathbb{N}}$, $j \in \mathbb{N}$, such that $\{u_k^{(j)}\}_{k\in\mathbb{N}} \subset \{u_k^{(j-1)}\}_{k\in\mathbb{N}}$ such that $\{\langle q_j\rangle^N a^W(x,hD)u_k^{(j)}(q_j)\}_{k\in\mathbb{N}}$ converges. Define $\{u_k'\}_{k\in\mathbb{N}}$ by $u_k' := u_k^{(k)}$, then $\{\langle q\rangle^N a^W(x,hD)u_k'(q)\}_{k\in\mathbb{N}}$ converges for all $q \in \mathbb{Q}^n$.

Let $\epsilon > 0$. Our goal is to show that there is some $K \in \mathbb{N}$ such that for all $k, l \geq K$ and all $x \in \mathbb{R}^n$, $|\langle x\rangle^N a^W(x,hD)u_k'(x) - \langle x\rangle^N a^W(x,hD)u_l'(x)| < \epsilon$. Choose $N > n/2$, and let α, β be multi-indices. Due to $a \in \mathscr{S}(\mathbb{R}^{2n})$ there exists some $C > 0$ s.t.

$$\begin{aligned}\sup_{x\in\mathbb{R}^n} |x^\alpha \partial^\beta (a^W(x,hD)u)| &\leq \sup_{(x,y)\in\mathbb{R}^{2n}} |x^\alpha \partial_x^\beta \langle y\rangle^N K(x,y)| \int_{\mathbb{R}^n} dy \left[\langle y\rangle^{-N}|u(y)|\right] \\ &\leq C\|u\|_{L^2},\end{aligned}$$

where we used the Cauchy-Schwartz inequality. The sequence $\{u_k'\}_{k\in\mathbb{N}}$ is bounded in the L^2-norm, so there is some $M > 0$ such that for all $k \in \mathbb{N}$, $x \in \mathbb{R}^n$,

$$|\partial\langle x\rangle^N a^W(x,hD)u_k'(x)| < M/3, \qquad \langle x\rangle^{N+1}|a^W(x,hD)u_k'(x)| < M/2.$$

We will consider two cases: where x is inside some open neighbourhood of 0, and where x is far away from 0. Let $R > 0$ be large enough such that $M/R \leq \epsilon$. Then

$$\begin{aligned}&\sup_{|x|\geq R} |\langle x\rangle^N a^W(x,hD)u_k'(x) - \langle x\rangle^N a^W(x,hD)u_l'(x)| \\ &\leq R^{-1} \sup_{|x|\geq R} |\langle x\rangle^{N+1} a^W(x,hD)u_k'(x)| + R^{-1} \sup_{|x|\geq R} |\langle x\rangle^{N+1} a^W(x,hD)u_l'(x)| \\ &< M/R < \epsilon.\end{aligned}$$

Finally, $\{B(q,\epsilon/M)\}_{q\in\mathbb{Q}^n}$ is an open cover of $\overline{B(0,R)}$, and so there is a finite subcover $\{B(q_p,\epsilon/M)\}_{1\leq p\leq P}$. For all $1 \leq p \leq P$, $\{\langle q_p\rangle^N a^W(x,hD)u_k'(q_p)\}_{k\in\mathbb{N}}$ converges. So there is some $K \in \mathbb{N}$ such that for all $k, l \geq K$, $1 \leq p \leq P$,

$$|\langle q_p\rangle^N a^W(x,hD)u_k'(q_p) - \langle q_p\rangle^N a^W(x,hD)u_l'(q_p)| < \epsilon/3.$$

For any $x \in B(0,R)$, choose $1 \leq p \leq P$ such that $x - q_p < \epsilon/M$, then for all $k, l \geq K$;

$$\begin{aligned}&|\langle x\rangle^N a^W(x,hD)u_k'(x) - \langle x\rangle^N a^W(x,hD)u_l'(x)| \\ &\quad\leq |\langle x\rangle^N a^W(x,hD)u_k'(x) - \langle q_p\rangle^N a^W(x,hD)u_k'(q_p)| \\ &\qquad + |\langle q_p\rangle^N a^W(x,hD)u_k'(q_p) - \langle q_p\rangle^N a^W(x,hD)u_l'(q_p) \\ &\qquad + |\langle x\rangle^N a^W(x,hD)u_l'(x) - \langle q_p\rangle^N a^W(x,hD)u_l'(q_p)| \\ &\quad< \epsilon/3 + |x - q_p|(\sup_x |\partial\langle x\rangle^N a^W(x,hD)u_k'(x)| + \sup_x |\partial\langle x\rangle^N a^W(x,hD)u_l'(x)|) \\ &\quad< \epsilon.\end{aligned}$$

□

Proposition 4.8. *(Formal adjoint) Let $t \in [0,1]$ and let $a \in \mathscr{S}(\mathbb{R}^{2n})$. Then the formal adjoint of $Op_t(a)$ is $Op_{1-t}(\overline{a})$, i.e. for all $u, v \in L^2(\mathbb{R}^n)$,*

$$\begin{aligned}\langle u, Op_t(a)v\rangle = \int_{\mathbb{R}^n} dx \left[\overline{u(x)} Op_t(a)v(x)\right] &= \int_{\mathbb{R}^n} dx \left[\overline{Op_{1-t}(\overline{a})u(x)} v(x)\right] \\ &= \langle Op_{1-t}(\overline{a})u, v\rangle.\end{aligned}$$

Proof. Let K_t be the kernel of $Op_t(a)$, then its complex conjugate is

$$\begin{aligned}\overline{K_t(x,y)} &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{a(tx + (1-t)y, \xi) e^{-\frac{i}{h}\langle x-y,\xi\rangle}}\right] \\ &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \left[\overline{a((1-t)y + (1-(1-t))x, \xi)} e^{\frac{i}{h}\langle y-x,\xi\rangle}\right],\end{aligned}$$

which is precisely the kernel of $Op_{1-t}(\overline{a})$. Hence

$$\begin{aligned}\langle u, Op_t(a)v\rangle &= \int_{\mathbb{R}^n} dx \left[\overline{u(x)} Op_t(a)v(x)\right] = \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} dy \left[\overline{u(x)} K_t(x,y)v(y)\right] \\ &= \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} dy \left[\overline{\overline{K_t(x,y)}u(x)}v(y)\right] = \int_{\mathbb{R}^n} dy \left[\overline{Op_{1-t}(\overline{a})u(y)}v(y)\right] \\ &= \langle Op_{1-t}(\overline{a})u, v\rangle.\end{aligned}$$

□

Lemma 4.9. *Let $a \in \mathscr{S}'(\mathbb{R}^n \times \mathbb{R}^n)$, then $Op_t(a) : \mathscr{S} \to \mathscr{S}'$.*

Proof. If $a \in \mathscr{S}'(\mathbb{R}^n \times \mathbb{R}^n)$, then $K_t \in \mathscr{S}'(\mathbb{R}^n \times \mathbb{R}^n)$. Now let $u, v \in \mathscr{S}(\mathbb{R}^n)$ and define $v \otimes u \in \mathscr{S}(\mathbb{R}^n \times \mathbb{R}^n)$ by $v \otimes u(x,y) := v(x)u(y)$. Then we can define $Op_t(a)u \in \mathscr{S}'(\mathbb{R}^n)$ by $Op_t(a)u(v) := K_t(v \otimes u)$. □

4.2 Composition of the Weyl quantisation

Let a, b be symbols, then we can ask what should be the symbol c such that $c^W(x,hD) = a^W(x,hD)b^W(x,hD)$. We will denote this symbol by $a\#b := c$. In this subsection, we will prove that

$$a\#b(z) = e^{\frac{i}{2h}\sigma(hD_z,hD_w)}(a(z)b(w))|_{z=w}.$$

In order to prove this, we will decompose symbols into Fourier components. The following lemmas will be useful.

Definition 4.10. *(Linear symbols) A symbol l of the form $l(z) := \langle z^*, z\rangle = \langle x^*, x\rangle + \langle \xi^*, \xi\rangle$ for some $z^* = (x^*, \xi^*) \in \mathbb{R}^{2n}$ is called a linear symbol. We will identify linear symbols l with their point $z^* \in \mathbb{R}^{2n}$.*

Now let $a \in \mathscr{S}(\mathbb{R}^{2n})$, then its semiclassical Fourier transform and its inverse are

$$\hat{a}_h(l) = \int_{\mathbb{R}^{2n}} dz \left[a(z)e^{-\frac{i}{h}l(z)}\right], \qquad a(z) = \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} dl \left[\hat{a}_h(l)e^{\frac{i}{h}l(z)}\right],$$

and so the quantisation is

$$Op_t(a) = \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} dl \left[\hat{a}_h(l) Op_t\left(e^{\frac{i}{h}l(\cdot)}\right)\right].$$

for all $t \in [0,1]$. The following lemmas deal with the quantisation and composition of such exponentials.

Lemma 4.11. *(Quantisation of linear symbols) Consider the linear symbol $l(x,\xi) := \langle x^*, x\rangle + \langle \xi^*, \xi\rangle$, then we have for all $t \in [0,1]$ that*

$$Op_t(l)u(x) = (\langle x^*, x\rangle + \langle \xi^*, hD\rangle)u(x) \tag{4.2}$$

Proof. This is just a simple calculation.

$$\begin{aligned}Op_t(l)u(x) &= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle} l(tx + (1-t)y, \xi)u(y)\right] \\ &= t\langle x^*, x\rangle u(x) + (1-t)\mathscr{F}_h^{-1} \circ \mathscr{F}_h(\langle x^*, \cdot\rangle u(\cdot))(x) + \mathscr{F}_h^{-1}(\langle \xi^*, \cdot\rangle \hat{u}_h(\cdot))(x) \\ &= \langle x^*, x\rangle u(x) + \langle \xi^*, hD_x\rangle u(x).\end{aligned}$$

□

Lemma 4.12. *(Quantisation of exponentials of linear symbols) Let l be a linear symbol, and define the symbol $a(z) := e^{\frac{i}{h}l(z)}$. Then we have*

$$Op_t(a)u(x) := e^{\frac{i}{h}\langle x^*, x\rangle + \frac{i}{h}(1-t)\langle x^*, \xi^*\rangle} u(x + \xi^*). \tag{4.3}$$

for all $t \in [0,1]$.

Proof. Again, we can simply calculate

$$\begin{aligned}
Op_t(a)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle} e^{\frac{i}{h}l(tx+(1-t)y,\xi)}u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle} e^{\frac{i}{h}\langle x^*,tx+(1-t)y\rangle+\frac{i}{h}\langle \xi^*,\xi\rangle}u(y)\right] \\
&= e^{\frac{i}{h}t\langle x^*,x\rangle}\frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x+\xi^*-y,\xi\rangle} e^{\frac{i}{h}(1-t)\langle x^*,y\rangle}u(y)\right] \\
&= e^{\frac{i}{h}t\langle x^*,x\rangle} e^{\frac{i}{h}(1-t)\langle x^*,x+\xi^*\rangle}u(x+\xi^*) \\
&= e^{\frac{i}{h}\langle x^*,x\rangle+\frac{i}{h}(1-t)\langle x^*,\xi^*\rangle}u(x+\xi^*).
\end{aligned}$$

□

Remark 4.13. *We can write*

$$e^{\frac{i}{h}l(x,hD)}u(x) = e^{\frac{i}{h}(\langle x^*,x\rangle+\frac{1}{2}\langle x^*,\xi^*\rangle)}u(x+\xi^*),$$

so that

$$\left(e^{\frac{i}{h}l(\cdot)}\right)^W(x,hD) = e^{\frac{i}{h}l(x,hD)} \tag{4.4}$$

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$ and $t \in \mathbb{R}$. The partial differential equation $\frac{h}{i}\partial_t v(x,t) = l(x,hD)v(x,t)$ with boundary condition $v(x,0) = u(x)$ has a unique solution, but it is solved by

$$v(x,t) = e^{\frac{it}{h}l(x,hD)}u(x)$$

as well as by

$$v(x,t) = e^{\frac{i}{h}(t\langle x^*,x\rangle+\frac{t^2}{2}\langle x^*,\xi^*\rangle)}u(x+t\xi^*),$$

□

hence these expressions must coincide.

We will now find $a\#b$ for exponentials of linear symbols. Then we can generalise this to arbitrary $a, b \in \mathscr{S}(\mathbb{R}^{2n})$ by using the Fourier decomposition of a and b.

Lemma 4.14. *(Composition of exponentials of linear symbols) Let $l, m \in \mathscr{S}(\mathbb{R}^{2n})$ be linear, i.e. $l = (x_1^*, \xi_1^*)$ and $m = (x_2^*, \xi_2^*)$ for some $(x_1^*, \xi_1^*), (x_2^*, \xi_2^*) \in \mathbb{R}^{2n}$, then*

$$e^{\frac{i}{h}l(x,hD)}e^{\frac{i}{h}m(x,hD)} = e^{\frac{i}{2h}\sigma(l,m)}e^{\frac{i}{h}(l+m)(x,hD)}, \tag{4.5}$$

where $\sigma(l,m) := \langle x_2^*, \xi_1^*\rangle - \langle x_1^*, \xi_2^*\rangle$ is the standard symplectic product on $\mathbb{R}^{2n}$.

Proof.

$$\begin{aligned}
e^{\frac{i}{h}l(x,hD)}e^{\frac{i}{h}m(x,hD)}u(x) &= e^{\frac{i}{h}l(x,hD)}e^{\frac{i}{h}\langle x_2^*,x+\frac{1}{2}\xi_2^*\rangle}u(x+\xi_2^*) \\
&= e^{\frac{i}{h}\langle x_1^*,x+\frac{1}{2}\xi_1^*\rangle}e^{\frac{i}{h}\langle x_2^*,x+\xi_1^*+\frac{1}{2}\xi_2^*\rangle}u(x+\xi_2^*+\xi_1^*) \\
&= e^{\frac{i}{2h}(\langle x_2^*,\xi_1^*\rangle-\langle x_1^*,\xi_2^*\rangle)}e^{\frac{i}{h}\langle x_1^*+x_2^*,x+\frac{1}{2}\xi_1^*+\frac{1}{2}\xi_2^*\rangle}u(x+\xi_1^*+\xi_2^*)b \\
&= e^{\frac{i}{2h}\sigma(l,m)}e^{\frac{i}{h}(l+m)(x,hD)}.
\end{aligned}$$

□

Theorem 4.15. *(Fourier decomposition of a^W) Let $a \in \mathscr{S}(\mathbb{R}^{2n})$ and $l \in \mathbb{R}^{2n}$, then*

$$a^W(x,hD) = \frac{1}{(2\pi h)^{2n}}\int_{\mathbb{R}^{2n}} dl \left[\hat{a}_h(l)e^{\frac{i}{h}l(x,hD)}\right]. \tag{4.6}$$

Moreover, if $a \in \mathscr{S}'(\mathbb{R}^{2n})$ and $u, v \in \mathscr{S}(\mathbb{R}^n)$, then we can view $e^{\frac{i}{h}l(x,hD)}u$ as a tempered distribution by setting

$$e^{\frac{i}{h}l(x,hD)}u(v) := \int_{\mathbb{R}^n} dx \left[e^{\frac{i}{h}l(x,hD)}u(x)v(x)\right],$$

which is itself in $\mathscr{S}(\mathbb{R}^{2n})$ as a function of l, so

$$a^W(x,hD)(u)(v) = \frac{1}{(2\pi h)^{2n}}\hat{a}_h\left(l \mapsto e^{\frac{i}{h}l(x,hD)}u(v)\right). \tag{4.7}$$

Theorem 4.16. *(Composition) Let $a, b \in \mathscr{S}(\mathbb{R}^{2n})$, then the symbol $a\#b$ defined by*

$$a\#b(z) := e^{\frac{i}{2h}\sigma(hD_z, hD_w)}(a(z)b(w))|_{z=w} \tag{4.8}$$

satisfies

$$(a\#b)^W(x, hD) = a^W(x, hD)b^W(x, hD). \tag{4.9}$$

Proof. Recall that $\sigma(hD_z, hD_w) = \langle hD_\xi, hD_y\rangle - \langle hD_\eta, hD_x\rangle$, so

$$\begin{aligned}
&e^{\frac{i}{2h}\sigma(hD_z,hD_w)}e^{\frac{i}{h}(l(z)+m(w))}\\
&= \sum_{k=0}^{\infty}\left[\frac{1}{k!}\left(\frac{i}{2h}\right)^k \sigma(hD_z, hD_w)^k e^{\frac{i}{h}(l(z)+m(w))}\right]\\
&= \sum_{k=0}^{\infty}\left[\frac{1}{k!}\left(\frac{i}{2h}\right)^k (\langle hD_\xi, hD_y\rangle - \langle hD_\eta, hD_x\rangle)^k e^{\frac{i}{h}(l(z)+m(w))}\right]\\
&= \sum_{k=0}^{\infty}\left[\frac{1}{k!}\left(\frac{i}{2h}\right)^k e^{\frac{i}{h}(l(z)+m(w))}(\langle \xi_1^*, x_2^*\rangle - \langle \xi_2^*, x_1^*\rangle)^k\right]\\
&= \sum_{k=0}^{\infty}\left[\frac{1}{k!}\left(\frac{i}{2h}\right)^k \sigma(l, m)^k e^{\frac{i}{h}(l(z)+m(w))}\right]\\
&= e^{\frac{i}{2h}\sigma(l,m)}e^{\frac{i}{h}(l(z)+m(w))}.
\end{aligned}$$

Using the Fourier decomposition of a and b, $a\#b$ can be written as

$$\begin{aligned}
&a\#b(z)\\
&= \frac{1}{(2\pi h)^{4n}}\int_{\mathbb{R}^{2n}} dl \int_{\mathbb{R}^{2n}} dm \left[e^{\frac{i}{2h}\sigma(hD_z,hD_w)}e^{\frac{i}{h}(l(z)+m(w))}|_{z=w}\hat{a}_h(l)\hat{b}_h(m)\right]\\
&= \frac{1}{(2\pi h)^{4n}}\int_{\mathbb{R}^{2n}} dl \int_{\mathbb{R}^{2n}} dm \left[e^{\frac{i}{2h}\sigma(l,m)}e^{\frac{i}{h}(l+m)(z)}\hat{a}_h(l)\hat{b}_h(m)\right],
\end{aligned}$$

so its Weyl quantisation becomes

$$\begin{aligned}
&(a\#b)^W(x, hD)\\
&= \frac{1}{(2\pi h)^{4n}}\int_{\mathbb{R}^{2n}} dl \int_{\mathbb{R}^{2n}} dm \left[e^{\frac{i}{2h}\sigma(l,m)}e^{\frac{i}{h}(l+m)(x,hD)}\hat{a}_h(l)\hat{b}_h(m)\right]\\
&= \frac{1}{(2\pi h)^{4n}}\int_{\mathbb{R}^{2n}} dl \int_{\mathbb{R}^{2n}} dm \left[e^{\frac{i}{h}l(x,hD)}e^{\frac{i}{h}m(x,hD)}\hat{a}_h(l)\hat{b}_h(m)\right]\\
&= a^W(x, hD)b^W(x, hD).
\end{aligned}$$

□

Symbols of the form $a(x, \xi) = a(\xi) = \sum_\alpha c_\alpha \xi^\alpha$ for certain constants c_α have the property that

$$\begin{aligned}
Op_t(a)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[\sum_\alpha c_\alpha \xi^\alpha u(y) e^{\frac{i}{h}\langle x-y,\xi\rangle}\right]\\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \left[\sum_\alpha c_\alpha \xi^\alpha \hat{u}_h(\xi) e^{\frac{i}{h}\langle x,\xi\rangle}\right]\\
&= \sum_\alpha c_\alpha (hD)^\alpha u(x).
\end{aligned}$$

This allows us to write equation (4.8) in integral form.

Lemma 4.17. *(Integral form of $a\#b$) Let $a, b \in \mathscr{S}(\mathbb{R}^{2n})$ and $z \in \mathbb{R}^{2n}$, then*

$$a\#b(z) = \frac{1}{(\pi h)^{2n}}\int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[e^{-\frac{2i}{h}\sigma(w_1,w_2)}a(z + w_1)b(z + w_2)\right] \tag{4.10}$$

Proof. Let $(w_1, w_2) = (y_1, \eta_1, y_2, \eta_2) \in \mathbb{R}^{4n}$ take the role of y, and let $(z, w) = (x, \xi, y, \eta) \in \mathbb{R}^{4n}$ the role of x, and $(z', w') \in \mathbb{R}^{4n}$ take the role of ξ. Then

$$\begin{aligned}
a\#b(z) &= e^{\frac{i}{2h}\sigma(hD_z, hD_w)}(a(z)b(w))|_{z=w} \\
&= \frac{1}{(2\pi h)^{4n}} \int_{\mathbb{R}^{4n}} d(w_1, w_2) \int_{\mathbb{R}^{4n}} d(z', w') \left[e^{\frac{i}{2h}\sigma(z', w')} e^{\frac{i}{h}\langle (z,w)-(w_1,w_2),(z',w')\rangle} a(w_1)b(w_2) \right]\Big|_{z=w} \\
&= \int_{\mathbb{R}^{4n}} d(w_1, w_2) \left[\mathscr{F}_h^{-1}\left((z', w') \mapsto e^{\frac{i}{2h}\sigma(z', w')} \right)(z - w_1, z - w_2) a(w_1) b(w_2) \right] \\
&= \int_{\mathbb{R}^{4n}} d(w_1, w_2) \left[\mathscr{F}_h^{-1}\left((z', w') \mapsto e^{\frac{i}{2h}\sigma(z', w')} \right)(-w_1, -w_2) a(z + w_1) b(z + w_2) \right],
\end{aligned}$$

where the inverse Fourier transform is given by

$$\begin{aligned}
&\mathscr{F}_h^{-1}\left((z, w) \mapsto e^{\frac{i}{2h}\sigma(z,w)} \right)(w_1, w_2) = \frac{1}{(2\pi h)^{4n}} \int_{\mathbb{R}^{4n}} d(z, w) \left[e^{\frac{i}{2h}\sigma(z,w)} e^{\frac{i}{h}\langle (w_1,w_2),(z,w)\rangle} \right] \\
&= \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} d(x, \eta) \left[e^{-\frac{i}{2h}\langle x, \eta\rangle} e^{\frac{i}{h}\langle x, y_1\rangle} e^{\frac{i}{h}\langle \eta, \eta_2\rangle} \right] \\
&\qquad \cdot \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} d(y, \xi) \left[e^{\frac{i}{2h}\langle y, \xi\rangle} e^{\frac{i}{h}\langle y, y_2\rangle} e^{\frac{i}{h}\langle \xi, \eta_1\rangle} \right] \\
&= \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{n}} d\eta \left[e^{\frac{i}{h}\langle \eta, \eta_2\rangle} \int_{\mathbb{R}^{n}} dx \left[e^{\frac{i}{h}\langle \frac{x}{2}, 2y_1\rangle} e^{-\frac{i}{h}\langle \frac{x}{2}, \eta\rangle} \right] \right] \\
&\qquad \cdot \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{n}} dy \left[e^{\frac{i}{h}\langle y, y_2\rangle} \int_{\mathbb{R}^{n}} d\xi \left[e^{\frac{i}{h}\langle \frac{\xi}{2}, 2\eta_1\rangle} e^{\frac{i}{h}\langle y, \frac{\xi}{2}\rangle} \right] \right] \\
&= \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{n}} d\eta \left[2^n \mathscr{F}_h\left(x \mapsto e^{\frac{i}{h}\langle x, 2y_1\rangle} \right)(\eta) e^{\frac{i}{h}\langle \eta, \eta_2\rangle} \right] \\
&\qquad \cdot \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{n}} dy \left[2^n \mathscr{F}_h^{-1}\left(\xi \mapsto e^{\frac{i}{h}\langle \xi, 2\eta_1\rangle} \right)(y) e^{-\frac{i}{h}\langle y, -y_2\rangle} \right] \\
&= \frac{1}{(\pi h)^n} e^{\frac{2i}{h}\langle y_2, \eta_1\rangle} \cdot \frac{1}{(\pi h)^n} e^{-\frac{2i}{h}\langle y_2, \eta_1\rangle} = \frac{1}{(\pi h)^{2n}} e^{\frac{2i}{h}\sigma(w_1, w_2)}. \qquad \square
\end{aligned}$$

Corollary 4.18. *($\#$ is associative) Let $a, b, c \in \mathscr{S}(\mathbb{R}^{2n})$, then $(a\#b)\#c = a\#(b\#c)$.*

Proof. Using the integral form, we obtain:

$$\begin{aligned}
(a\#b)\#c(z) &= \frac{1}{(2\pi h)^{4n}} \int_{\mathbb{R}^{8n}} d\tilde{w_1} d\tilde{w_2} dw_1 dw_2 \left[e^{-\frac{2i}{h}(\sigma(\tilde{w_1}, \tilde{w_2}) + \sigma(w_1, w_2))} a(z + \tilde{w_1} + w_1) b(z + \tilde{w_1} + w_2) c(z + \tilde{w_2}) \right] \\
a\#(b\#c)(z) &= \frac{1}{(2\pi h)^{4n}} \int_{\mathbb{R}^{8n}} d\tilde{v_1} d\tilde{v_2} dv_1 dv_2 \left[e^{-\frac{2i}{h}(\sigma(\tilde{v_1}, \tilde{v_2}) + \sigma(v_1, v_2))} a(z + \tilde{v_1}) b(z + \tilde{v_2} + v_1) c(z + \tilde{v_2} + v_2) \right]
\end{aligned}$$

It is easy to see that these integrals are equal by using the substitution $v_1 = \tilde{w_1}, v_2 = \tilde{w_2} - w_2, \tilde{v_1} = \tilde{w_1} + w_1, \tilde{v_2} = w_2$. $\square$

Definition 4.19. *Let $\varphi \in \mathscr{S}(\mathbb{R}^n), N \in \mathbb{N}$, then we say $\varphi = O_{\mathscr{S}}(h^N)$ if for all multi-indices α, β, there is a constant $C_{\alpha,\beta} > 0$ such that*

$$\sup_{x \in \mathbb{R}^n} |x^\alpha \partial^\beta \varphi(x)| \leq C_{\alpha,\beta} h^N$$

as $h \to 0$.

Theorem 4.20. *Let $a, b \in \mathscr{S}(\mathbb{R}^{2n})$, and $N \in \mathbb{N}$, then*

$$a\#b(z) = \sum_{k=0}^{N-1} \left[\frac{1}{k!} \left(\frac{ih}{2} \right)^k \sigma(D_z, D_w)^k (a(z)b(w)) \right]\Big|_{z=w} + O_{\mathscr{S}}(h^N) \tag{4.11}$$

as $h \to 0$.

Proof. First note that

$$\mathscr{F}^{-1}\left((z,w)\mapsto e^{-\frac{2i}{h}\sigma(z,w)}\right)(w_1,w_2)=\left(\frac{h}{4\pi}\right)^{2n}e^{\frac{ih}{2}\sigma(w_1,w_2)},$$

the proof of which is similar to the calculation in the previous lemma. Now we have for all $z\in\mathbb{R}^{2n}$,

$$\begin{aligned}
a\#b(z)&=\frac{1}{(\pi h)^{2n}}\int_{\mathbb{R}^{2n}}dw_1\int_{\mathbb{R}^{2n}}dw_2\left[e^{-\frac{2i}{h}\sigma(w_1,w_2)}a(z+w_1)b(z+w_2)\right]\\
&=\frac{1}{(\pi h)^{2n}}\int_{\mathbb{R}^{2n}}dw_1\int_{\mathbb{R}^{2n}}dw_2\left[\mathscr{F}^{-1}\left((z,w)\mapsto e^{-\frac{2i}{h}\sigma(z,w)}\right)(w_1,w_2)e^{i\langle z,w_1+w_2\rangle}\hat{a}(w_1)\hat{b}(w_2)\right]\\
&=\frac{1}{(2\pi)^{4n}}\int_{\mathbb{R}^{2n}}dw_1\int_{\mathbb{R}^{2n}}dw_2\left[e^{\frac{ih}{2}\sigma(w_1,w_2)}e^{i\langle z,w_1+w_2\rangle}\hat{a}(w_1)\hat{b}(w_2)\right]\\
&=\frac{1}{(2\pi)^{4n}}\int_{\mathbb{R}^{2n}}dw_1\int_{\mathbb{R}^{2n}}dw_2\left[e^{i(\frac{h}{2}\sigma(w_1,w_2)+\langle z,w_1+w_2\rangle)}\mathscr{F}(a\otimes b)(w_1,w_2)\right].
\end{aligned}$$

We will introduce the convenient notation $J_z(h,a\otimes b):=a\#b(z)$ as well as $P:=\frac{i}{2}\sigma(D_{w_1'},D_{w_2'})$. Then

$$\begin{aligned}
&\partial_h J_z(h,a\otimes b)\\
&=\frac{1}{(2\pi)^{4n}}\int_{\mathbb{R}^{4n}}d(w_1,w_2)\left[e^{i(\frac{h}{2}\sigma(w_1,w_2)+\langle z,w_1+w_2\rangle)}\frac{i}{2}\sigma(w_1,w_2)\mathscr{F}(a\otimes b)(w_1,w_2)\right]\\
&=\frac{1}{(2\pi)^{4n}}\int_{\mathbb{R}^{4n}}d(w_1,w_2)\left[e^{i(\frac{h}{2}\sigma(w_1,w_2)+\langle z,w_1+w_2\rangle)}\mathscr{F}(Pa\otimes b)(w_1,w_2)\right]\\
&=J_z(h,Pa\otimes b)
\end{aligned}$$

Consequently, $\partial_h^k J_z(h,a\otimes b)=J_z(h,P^k a\otimes b)$ for all $k\in\mathbb{N}$. Taylor's theorem around $h=0$ now gives for any $N\in\mathbb{N}$ that

$$a\#b(z)=\sum_{k=0}^{N-1}\left[\frac{h^k}{k!}J_z(0,P^k a\otimes b)\right]+\frac{h^N}{N!}R_{z,N}(h,a\otimes b)$$

where $R_{z,N}(h,a\otimes b):=N\int_0^1 dt[(1-t)^{N-1}J_z(th,P^N a\otimes b)]$. It is now left to show that $J_z(0,P^k a\otimes b)$ is indeed the required expression and that the rest term is indeed $O_{\mathscr{S}}(h^N)$, i.e. $|R_{z,N}(h,a\otimes b)|$ is bounded independent of h.

- $$\begin{aligned}
&J_z(0,P^k a\otimes b)\\
&=\frac{1}{(2\pi)^{4n}}\int_{\mathbb{R}^{4n}}d(w_1,w_2)\left[\mathscr{F}\left((w_1',w_2')\mapsto\left(\frac{i}{2}\right)^k\sigma(D_{w_1'},D_{w_2'})^k a(w_1')b(w_2')\right)(w_1,w_2)e^{i\langle z,w_1+w_2\rangle}\right]\\
&=\left(\frac{i}{2}\right)^k\sigma(D_z,D_w)^k a(z)b(w)\Big|_{z=w}
\end{aligned}$$
- $$\begin{aligned}
&|R_{z,N}(h,a\otimes b)|\\
&=\left|N\int_0^1 dt\left[(1-t)^{N_1}J_z(th,p^N a\otimes b)\right]\right|\leq C_N\|\mathscr{F}(P^N a\otimes b)\|_{L^1}\\
&\leq C_N\max_{|\alpha|\leq n+1}\|\partial^\alpha P^N a\otimes b\|_{L^1}\leq C_N\max_{|\alpha|\leq N+n+1}\|\partial^\alpha a\otimes b\|_{L^1},
\end{aligned}$$

by lemma 3.6. ☐

Corollary 4.21. *Let $a,b\in\mathscr{S}(\mathbb{R}^{2n})$, then*

$$a\#b=ab+\frac{h}{2i}\{a,b\}+O_{\mathscr{S}}(h^2)\tag{4.12}$$

and

$$[a^W(x,hD),b^W(x,hD)]=\frac{h}{i}\{a,b\}^W(x,hD)+O_{\mathscr{S}}(h^3)\tag{4.13}$$

where $[A,B]:=AB-BA$ is the commutator and $\{f,g\}:=\sum_{j=1}^n(f_{\xi_j}g_{x_j}-f_{x_j}g_{\xi_j})$ is the Poisson bracket on $C^\infty(\mathbb{R}^{2n})$.

Proof.

$$\begin{aligned}
&a\#b(z)\\
&= a(z)b(z) + \frac{ih}{2}\sigma(D_z, D_w)a(z)b(w)\Big|_{z=w} + O_{\mathscr{S}}(h^2)\\
&= a(z)b(z) + \frac{h}{2i}(\partial_y\partial_\xi - \partial_x\partial_\eta)a(x,\xi)b(y,\eta)\Big|_{(x,\xi)=(y,\eta)} + O_{\mathscr{S}}(h^2)\\
&= a(z)b(z) + \frac{h}{2i}\{a,b\}(z) + O_{\mathscr{S}}(h^2)\\
&[a^W(x,hD), b^W(x,hD)]\\
&= (a\#b)^W(x,hD) - (b\#a)^W(x,hD)\\
&= \frac{h}{i}\{a,b\}^W(x,hD) - \frac{h^2}{8}\sigma(D_z,D_w)^2(a(z)b(w) - b(z)a(w))\Big|_{z=w} + O_{\mathscr{S}}(h^3)\\
&= \frac{h}{i}\{a,b\}^W(x,hD) + O_{\mathscr{S}}(h^3)
\end{aligned}$$

□

4.3 Symbol classes

In this subsection we will prove that $a^W(x,hD) : L^2 \to L^2$ is well-defined as a bounded operator for certain symbol classes that are larger than $\mathscr{S}(\mathbb{R}^{2n})$.

Definition 4.22. *(Order functions) A measurable function $m : \mathbb{R}^{2n} \longrightarrow (0,\infty)$ is called an order function if $\exists C, N \in \mathbb{R}$ such that $\forall w, z \in \mathbb{R}^{2n}$,*

$$m(w) \leq C\langle z - w\rangle^N m(z),$$

where $\langle z\rangle := \sqrt{1+|z|^2}$.

Proposition 4.23. *Let m, m_1, and m_2 be order functions and let $a \in [0,\infty)$, then m^a, $1/m$, $m_1 + m_2$, and m_1m_2 are order functions as well. Moreover, $m_{k,l}$ defined by*

$$m_{k,l}(z) := \langle x\rangle^k + \langle\xi\rangle^l \tag{4.14}$$

is an order function for all $k, l \in \mathbb{R}$.

Proof. Since m is an order function, there are constants $C, N \in \mathbb{R}$ such that $m(w) \leq C\langle z-w\rangle^N m(z)$ for all $w, z \in \mathbb{R}^{2n}$. Then

$$\begin{aligned}
m^a(w) &\leq C^a\langle z-w\rangle^{Na}m^a(z), \text{ and}\\
\frac{1}{m(z)} &\leq C\langle z-w\rangle^N\frac{1}{m(w)}.
\end{aligned}$$

Now let $C_j, N_j \in \mathbb{R}$ such that $m_j(w) \leq C_j\langle z-w\rangle^{N_j}m_j(z)$ for $j = 1,2$ and all $w, z \in \mathbb{R}^{2n}$, and assume without loss of generality that $N_1 \leq N_2$. Then

$$\begin{aligned}
(m_1+m_2)(w) = m_1(w) + m_2(w) &\leq C_1\langle z-w\rangle^{N_1}m_1(z) + C_2\langle z-w\rangle^{N_2}m_2(z)\\
&= \langle z-w\rangle^{N_2}\left(C_1\langle z-w\rangle^{-(N_2-N_1)}m_1(z) + C_2m_2(z)\right)\\
&\leq \langle z-w\rangle^{N_2}\left(C_1m_1(z) + C_2m_2(z)\right)\\
&\leq \max(C_1,C_2)\langle z-w\rangle^{N_2}(m_1+m_2)(z),\\
(m_1m_2)(w) = m_1(w)m_2(w) &\leq C_1C_2\langle z-w\rangle^{N_1+N_2}(m_1m_2)(z).
\end{aligned}$$

Now it is only left to show that $m(w) := \langle x\rangle$ is an order function. Note that

$$\begin{aligned}
m(w) = \langle y\rangle = \sqrt{1+|y|^2} &\leq \sqrt{1+(|y-x|+|x|)^2}\\
&= \sqrt{1+|y-x|^2+|x|^2+2|x||y-x|}
\end{aligned}$$

We will consider two cases: (a) $|x||y-x| \le 1$, and (b) $|x||y-x| \ge 1$. Then

$$\begin{aligned}
m(w) &\overset{(a)}{\le} \sqrt{1+|x-y|^2+|x|^2+2} \le \sqrt{2}\sqrt{1+|x-y|^2+1+|x|^2} \\
&\le \sqrt{2}\left(\langle y-x\rangle + \langle x\rangle\right) \le 2\sqrt{2}\max(\langle y-x\rangle, \langle x\rangle) \\
&\le 2\sqrt{2}\langle y-x\rangle\langle x\rangle = 2\sqrt{2}\langle y-x\rangle m(z), \\
m(w) &\overset{(b)}{\le} \sqrt{1+|y-x|^2+|x|^2+2|y-x|^2|x|^2} \le \sqrt{2}\sqrt{(1+|y-x|^2)(1+|x|^2)} \\
&= \sqrt{2}\langle y-x\rangle\langle x\rangle = \sqrt{2}\langle y-x\rangle m(z).
\end{aligned}$$

□

Definition 4.24. *(Symbol classes) Let $m : \mathbb{R}^{2n} \to (0,\infty)$ be an order function and let $\delta \ge 0$, then*

$$S_\delta(m) := \{a \in C^\infty \mid \forall \alpha, \exists C_\alpha > 0; |\partial^\alpha a| \le C_\alpha h^{-\delta|\alpha|} m\}. \tag{4.15}$$

We shall write $S(m) := S_0(m)$, $S_\delta := S_\delta(1)$, and $S := S_0(1)$. Note that

$$\sup_{z,h} m < \infty \Longrightarrow S_\delta(m) \subseteq S_\delta,$$
$$\inf_{z,h} m > 0 \Longrightarrow S_\delta \subseteq S_\delta(m).$$

The constant $\delta \ge 0$ is relevant in case we want to study $a^W(x,hD)$ in the limit $h \to 0$. Of course, the quantisation formula (4.1) itself already depends on h. By rescaling $\tilde{x} := h^{-\frac{1}{2}}x$, $\tilde{\xi} := h^{-\frac{1}{2}}\xi$, $\tilde{y} := h^{-\frac{1}{2}}y$, $\tilde{u}(\tilde{x}) := u(x) = u(h^{\frac{1}{2}}\tilde{x})$, $\tilde{a}(\tilde{x},\tilde{\xi}) := a(x,\xi) = a(h^{\frac{1}{2}}\tilde{x}, h^{\frac{1}{2}}\tilde{\xi})$, we obtain

$$\begin{aligned}
a^W(x,hD)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle} a\left(\frac{x+y}{2},\xi\right) u(y)\right] \\
&= \frac{1}{(2\pi h)^n} h^n \int_{\mathbb{R}^n} d\tilde{\xi} \int_{\mathbb{R}^n} d\tilde{y} \left[e^{i\langle \tilde{x}-\tilde{y},\tilde{\xi}\rangle} a\left(h^{\frac{1}{2}}\frac{\tilde{x}+\tilde{y}}{2}, h^{\frac{1}{2}}\xi\right) u(h^{\frac{1}{2}}\tilde{y})\right] \\
&= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} d\tilde{\xi} \int_{\mathbb{R}^n} d\tilde{y} \left[e^{i\langle \tilde{x}-\tilde{y},\tilde{\xi}\rangle} \tilde{a}\left(\frac{\tilde{x}+\tilde{y}}{2},\tilde{\xi}\right) \tilde{u}(\tilde{y})\right] \\
&= \tilde{a}^W(\tilde{x},D)\tilde{u}(\tilde{x}).
\end{aligned}$$

Let $\delta \ge 0$, let m be an order function, and let $a \in S_\delta(m)$. Then for all multi-indices α, the rescaled function $\tilde{a}$ satisfies $|\partial^\alpha \tilde{a}| = h^{\frac{1}{2}|\alpha|}|\partial^\alpha a| \le C_\alpha h^{|\alpha|(\frac{1}{2}-\delta)} m$. This is unbounded as $h \to 0$ for $\delta > \frac{1}{2}$, so from now on we will always assume that $0 \le \delta \le \frac{1}{2}$.

Proposition 4.25. *Let $\delta \ge 0$ and $t \in [0,1]$. Let m be an order function, and let $a \in S_\delta(m)$. Then*

$$Op_t(a) : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$$

is a continuous linear operator.

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$. We want to prove that $x \mapsto Op_t(a)u(x)$ is again a Schwartz function. We will first prove that $\sup_{x\in\mathbb{R}^n} |Op_t(a)u(x)| < \infty$. Then, for $1 \le j \le n$, we will apply this to the cases $x_j Op_t(a)u(x)$ and $\partial_j Op_t(a)u(x)$ by writing these as the finite sum of functions of the form $Op_t(b)v(x)$ for certain $b \in S_\delta(m)$, $v \in \mathscr{S}(\mathbb{R}^n)$.

Let $C, N > 0$ such that $m(w) \le C\langle z-w\rangle^N m(z)$ for all $w, z \in \mathbb{R}^{2n}$. Then for all $1 \le j \le n$,

$$\begin{aligned}
hD_{y_j} e^{\frac{i}{h}\langle x-y,\xi\rangle} &= -\xi_j e^{\frac{i}{h}\langle x-y,\xi\rangle}, \text{ and} \\
hD_{\xi_j} e^{\frac{i}{h}\langle x-y,\xi\rangle} &= (x_j - y_j) e^{\frac{i}{h}\langle x-y,\xi\rangle}.
\end{aligned}$$

So for the operators L_1 and L_2 defined by

$$\begin{aligned}
L_1 &:= \frac{1-\langle \xi, hD_y\rangle}{1+|\xi|^2} = \frac{1-\langle \xi, hD_y\rangle}{\langle \xi\rangle^2}, \\
L_2 &:= \frac{1+\langle x-y, hD_\xi\rangle}{1+|x-y|^2} = \frac{1+\langle x-y, hD_\xi\rangle}{\langle x-y\rangle^2},
\end{aligned}$$

the identities $L_1 e^{\frac{i}{h}\langle x-y,\xi\rangle} = L_2 e^{\frac{i}{h}\langle x-y,\xi\rangle} = e^{\frac{i}{h}\langle x-y,\xi\rangle}$ hold. Then we obtain

$$\begin{aligned}
Op_t(a)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} d(\xi,y)\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}a\left(tx+(1-t)y,\xi\right)u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} d(\xi,y)\left[L_1^{N+n+1}\left(e^{\frac{i}{h}\langle x-y,\xi\rangle}\right)a\left(tx+(1-t)y,\xi\right)u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} d(\xi,y)\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right]
\end{aligned}$$

by integration by parts, where the boundary term vanishes because $u(y)$ is a Schwartz function,

$$\begin{aligned}
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} d(\xi,y)\left[L_2^{N+n+1}\left(e^{\frac{i}{h}\langle x-y,\xi\rangle}\right)\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} d(\xi,y)\Bigg[e^{\frac{i}{h}\langle x-y,\xi\rangle} \\
&\qquad \cdot\sum_{l=0}^{N+n+1}\frac{(-1)^l\langle x-y,hD_\xi\rangle^l}{\langle x-y\rangle^{2(N+n+1)}}\left[\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right]\Bigg]
\end{aligned}$$

by integration by parts where the boundary term vanishes because a and all its derivatives grow by at most $\sim\langle\xi\rangle^N$.

All derivatives of $a(tx+(1-t)y,\xi)u(y)$ grow by at most $\sim\langle x-y\rangle^N\langle\xi\rangle^N$, hence for some $C>0$,

$$\sup_{x\in\mathbb{R}^n}|Op_t(a)u(x)|\le C\int_{\mathbb{R}^n}d\xi\int_{\mathbb{R}^n}dy\left[\frac{1}{\langle x-y\rangle^{n+1}}\frac{1}{\langle\xi\rangle^{n+1}}\right]<\infty.$$

Now let $1\le j\le n$, then

$$\begin{aligned}
&(2\pi h)^n x_j Op_t(a)u(x) \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[x_j e^{\frac{i}{h}\langle x-y,\xi\rangle}\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right] \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[(y_j+hD_{\xi_j})\left(e^{\frac{i}{h}\langle x-y,\xi\rangle}\right)\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right] \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}(y_j-hD_{\xi_j})\sum_{k=0}^{N+n+1}\frac{\langle\xi,hD_y\rangle^k}{\langle\xi\rangle^{2(N+n+1)}}\left(a\left(tx+(1-t)y,\xi\right)u(y)\right)\right], \\
&(2\pi h)^n hD_{x_j}a^W(x,hD)u(x) \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[hD_{x_j}\left(e^{\frac{i}{h}\langle x-y,\xi\rangle}a\left(tx+(1-t)y,\xi\right)\right)u(y)\right] \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[\left(\xi_j e^{\frac{i}{h}\langle x-y,\xi\rangle}a\left(tx+(1-t)y,\xi\right)+e^{\frac{i}{h}\langle x-y,\xi\rangle}hD_{x_j}a\left(\frac{x+y}{2},\xi\right)\right)u(y)\right] \\
&\quad= \int_{\mathbb{R}^{2n}} d(\xi,y)\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\left[\frac{1+\langle\xi,hD_y\rangle}{\langle\xi\rangle^2}\left(\xi_j a\left(tx+(1-t)y,\xi\right)u(y)\right)+hD_{x_j}a\left(\frac{x+y}{2},\xi\right)u(y)\right]\right].
\end{aligned}$$

Now let $\{u_j\}_{j\in\mathbb{N}}\subset\mathscr{S}(\mathbb{R}^n)$ be a Cauchy sequence converging to 0, then it is clear from the above expressions that the sequence $Op_t(a)u_j$ also converges to 0 in $\mathscr{S}(\mathbb{R}^n)$, hence $Op_t(a)$ is continuous. □

Proposition 4.26. *Let $\delta\ge 0$, $t\in[0,1]$. Let m be an order function, and let $a\in S_\delta(m)$. Then*

$$Op_t(a):\mathscr{S}'(\mathbb{R}^n)\to\mathscr{S}'(\mathbb{R}^n)$$

is a continuous linear operator.

Proof. Let $u, v \in \mathscr{S}(\mathbb{R}^n)$ and define $\tilde{\xi} := -\xi$, $\tilde{a}(x, \tilde{\xi}) := a(x, \xi) = a(x, -\tilde{\xi})$, then

$$\begin{aligned}
&\int_{\mathbb{R}^n} dx \left[v(x) Op_t(a) u(x)\right] \\
&= \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} dx \int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y, \xi\rangle} a\left(tx + (1-t)y, \xi\right) u(y) v(x)\right] \\
&= \int_{\mathbb{R}^n} dy \left[u(y) \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^{2n}} d(\xi, x) \left[e^{\frac{i}{h}\langle y-x, -\xi\rangle} a\left(tx + (1-t)y, -(-\xi)\right) v(x)\right]\right] \\
&= \int_{\mathbb{R}^n} dy \left[u(y) \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^{2n}} d(\tilde{\xi}, x) \left[e^{\frac{i}{h}\langle y-x, \tilde{\xi}\rangle} a\left(tx + (1-t)y, -\tilde{\xi}\right) v(x)\right]\right] \\
&= \int_{\mathbb{R}^n} dy \left[u(y) \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^{2n}} d(\tilde{\xi}, x) \left[e^{\frac{i}{h}\langle y-x, \tilde{\xi}\rangle} \tilde{a}\left(tx + (1-t)y, \tilde{\xi}\right) v(x)\right]\right] \\
&= \int_{\mathbb{R}^n} dy \left[u(y) Op_t(\tilde{a}) v(y)\right],
\end{aligned}$$

so we can define for $u \in \mathscr{S}'(\mathbb{R}^n)$ and $v \in \mathscr{S}(\mathbb{R}^n)$ that

$$(Op_t(a)u)(v) := u(Op_t(\tilde{a})v).$$

□

So far, we have considered quantisation for symbols in $\mathscr{S}(\mathbb{R}^n)$ or in $S_\delta(m)$. We will now try to construct such a symbol for a given operator $A : \mathscr{S}' \to \mathscr{S}'$. It turns out that for all $t \in [0, 1]$ and all $a \in S_\delta(m)$, the identity

$$a(x, \xi) = e^{\frac{i}{h}(t-1)\langle hD_x, hD_\xi\rangle} \left(e^{-\frac{i}{h}\langle x, \xi\rangle} Op_t(a) \left(x \mapsto e^{\frac{i}{h}\langle x, \xi\rangle}\right)\right)(x) \tag{4.16}$$

holds. We will first prove this for standard quantisation, i.e. $t = 1$.

Lemma 4.27. *Let $0 \le \delta \le \frac{1}{2}$ and let m be an order function. Let $a \in S_\delta(m)$, then*

$$a(x, \xi) = e^{-\frac{i}{h}\langle x, \xi\rangle} a(x, hD) \left(x \mapsto e^{\frac{i}{h}\langle x, \xi\rangle}\right)(x). \tag{4.17}$$

Proof. Using example 3.9, we obtain

$$\begin{aligned}
&e^{-\frac{i}{h}\langle x, \xi\rangle} a(x, hD) \left(x \mapsto e^{\frac{i}{h}\langle x, \xi\rangle}\right)(x) \\
&= e^{-\frac{i}{h}\langle x, \xi\rangle} \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\eta \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y, \eta\rangle} a(x, \eta) e^{\frac{i}{h}\langle y, \xi\rangle}\right] \\
&= \int_{\mathbb{R}^n} d\eta \left[a(x, \eta) e^{\frac{i}{h}\langle x, \eta-\xi\rangle} \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle y, \eta-\xi\rangle}\right]\right] \\
&= \int_{\mathbb{R}^n} d\eta \left[a(x, \eta) e^{\frac{i}{h}\langle x, \eta-\xi\rangle} \delta_0(\eta - \xi)\right] \\
&= a(x, \xi).
\end{aligned}$$

□

Proposition 4.28. *Let $0 \le \delta \le \frac{1}{2}$ and let m be an order function. Let $b \in S_\delta(m)$ and define for $t \in [0, 1]$;*

$$a(x, \xi) := e^{-\frac{i}{h}(1-t)\langle hD_x, hD_\xi\rangle} b(x, \xi).$$

Then $a \in S_\delta(m)$ and $Op_t(a) = Op_1(b) = b(x, hD)$. Moreover, if $b \in \mathscr{S}(\mathbb{R}^{2n})$, then also $a \in \mathscr{S}(\mathbb{R}^{2n})$.

Proof. The operator $e^{-\frac{i}{h}(1-t)\langle hD_x, hD_\xi\rangle}$ arises by quantisation from the symbol $A(z, z') = e^{-\frac{i}{h}(1-t)\langle x', \xi'\rangle}$, where $z = (x, \xi)$ takes the role of x, $z' = (x', \xi')$ takes the role of ξ, and $w = (y, \eta)$ takes the role of y, i.e.

$$\begin{aligned}
&e^{-\frac{i}{h}(1-t)\langle hD_x, hD_\xi\rangle} b(x,\xi)\\
&= \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} dz' \int_{\mathbb{R}^{2n}} dw \left[e^{\frac{i}{h}\langle z-w, z'\rangle} e^{-\frac{i}{h}(1-t)\langle x', \xi'\rangle} b(w)\right]\\
&= \frac{1}{(2\pi h)^{2n}} \int_{\mathbb{R}^{2n}} d(\xi',\eta) \int_{\mathbb{R}^{2n}} d(x',y) \left[e^{\frac{i}{h}\langle x-y, x'\rangle} e^{\frac{i}{h}\langle \xi-\eta, \xi'\rangle} e^{-\frac{i}{h}(1-t)\langle x', \xi'\rangle} b(y,\eta)\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} d(\xi',\eta) \left[\frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} d(x',y) \left[e^{\frac{i}{h}\langle x-(1-t)\xi'-y, x'\rangle} e^{\frac{i}{h}\langle \xi-\eta, \xi'\rangle} b(y,\eta)\right]\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} d(\xi',\eta) \left[e^{\frac{i}{h}\langle \xi-\eta, \xi'\rangle} b(x-(1-t)\xi', \eta)\right].
\end{aligned}$$

Now we can define

$$\begin{aligned}
L_1 &:= \frac{1-\langle \xi', hD_\eta\rangle}{1+|\xi'|^2} = \frac{1-\langle \xi', hD_\eta\rangle}{\langle \xi'\rangle^2},\\
L_2 &:= \frac{1+\langle \xi-\eta, hD_{\xi'}\rangle}{1+|\xi-\eta|^2} = \frac{1+\langle \xi-\eta, hD_{\xi'}\rangle}{\langle \xi-\eta\rangle^2},
\end{aligned}$$

so that $L_1 e^{\frac{i}{h}\langle \xi-\eta,\xi'\rangle} = L_2 e^{\frac{i}{h}\langle \xi-\eta,\xi'\rangle} = e^{\frac{i}{h}\langle \xi-\eta,\xi'\rangle}$. Now we can use arguments similar to those in the proof of proposition 4.25 to show that $b \in \mathscr{S}(\mathbb{R}^{2n}) \implies a \in \mathscr{S}(\mathbb{R}^{2n})$ and $b \in S_\delta(m) \implies a \in S_\delta(m)$.

Now let $b \in \mathscr{S}(\mathbb{R}^{2n})$ and $u \in \mathscr{S}(\mathbb{R}^n)$, then

$$\begin{aligned}
&Op_t(a)u(x)\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} dl \left[\hat{a}_h(l)\, Op_t\left(e^{\frac{i}{h}l(\cdot)}\right) u(x)\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} dl \left[\mathscr{F}_h\left(e^{-\frac{i}{h}}(1-t)\langle hD_x, hD_\xi\rangle b(x,\xi)\right)(l)\, Op_t\left(e^{\frac{i}{h}l(\cdot)}\right) u(x)\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} dl \left[e^{-\frac{i}{h}(1-t)\langle x^*, \xi^*\rangle} \hat{b}_h(l) e^{\frac{i}{h}\langle x^*, x\rangle + \frac{i}{h}(1-t)\langle x^*,\xi^*\rangle} u(x+\xi^*)\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} dl \left[\hat{b}_h(l) e^{\frac{i}{h}\langle x^*, x\rangle} u(x+\xi^*)\right]\\
&= \frac{1}{(2\pi h)^{n}} \int_{\mathbb{R}^{2n}} dl \left[\hat{b}_h(l) Op_1\left(e^{\frac{i}{h}l(\cdot)}\right) u(x)\right]\\
&= Op_1(b)u(x).
\end{aligned}$$

Using the fact that $\mathscr{S}(\mathbb{R}^{2n}) \subset S_\delta(m)$ is dense, we obtain $Op_t(a) = Op_1(b)$ for all $b \in S_\delta(m)$. ☐

Definition 4.29. *(Order of vanishing) Let $0 \le \delta \le \frac{1}{2}$ and let m be an order function. Then a function $a \in S_\delta(m)$ is said to vanish with order N as $h \to 0$ if for each multi-index α there is a constant $C > 0$ such that $|\partial^\alpha a| \le C h^{N-\delta|\alpha|} m$. If this is the case, we write $a = O_{S_\delta(m)}(h^N)$.*

Proposition 4.30. *(Composition) Let $0 \le \delta < \frac{1}{2}$ and let m_1 and m_2 be order functions. Let $a \in S_\delta(m_1), b \in S_\delta(m_2)$, then $a\#b \in S_\delta(m_1 m_2)$ and $a^W(x,hD)b^W(x,hD) = (a\#b)^W(x,hD)$. Moreover, for all $n \in \mathbb{N}$ we have*

$$a\#b(z) = \sum_{k=0}^{N-1} \left[\frac{1}{k!}\left(\frac{ih}{2}\right)^k \sigma(D_z, D_w)^k (a(z)b(w))\right]\Bigg|_{z=w} + O_{S_\delta(m_1 m_2)}(h^{k(1-2\delta)}). \tag{4.18}$$

Proof. Clearly, $(z,w) \mapsto a(z)b(w) \in S_\delta((z,w) \mapsto m_1(z)m_2(w))$. Now we need to prove that $e^{\frac{i}{2h}\sigma(hD_z, hD_w)} : S_\delta((z,w) \mapsto a(z)b(w)) \to S_\delta((z,w) \mapsto a(z)b(w))$. The proof of this is very similar to the previous proof, so it will be omitted. Then $a\#b := e^{\frac{i}{2h}\sigma(hD_z,hD_w)}(a(z)b(w))\Big|_{z=w} \in S_\delta(m_1 m_2)$.

Let α be a multi-index, then

$$\partial_z^\alpha \left(\frac{1}{k!} \left(\frac{ih}{2}\right)^k \sigma(D_z, D_w)^k (a(z)b(w)) \Big|_{z=w} \right) \leq h^k C h^{-(2k+|\alpha|)\delta} m_1 m_2 = C h^{k(1-2\delta)-\delta|\alpha|} m_1 m_2,$$

hence

$$\frac{1}{k!} \left(\frac{ih}{2}\right)^k \sigma(D_z, D_w)^k (a(z)b(w)) \Big|_{z=w} = O_{S_\delta(m_1 m_2)}(h^{k(1-2\delta)}). \qquad \square$$

Corollary 4.31. *If $a \in S_\delta(m_1)$ and $b \in S_\delta(m_2)$, then*

$$a\#b = ab + \frac{h}{2i}\{a, b\} + O_{S_\delta(m_1 m_2)}(h^{2(1-2\delta)}) \tag{4.19}$$

and

$$[a^W(x, hD), b^W(x, hD)] = \frac{h}{i}\{a, b\}^W(x, hD) + O_{\mathscr{S}'(\mathbb{R}^n) \to \mathscr{S}'(\mathbb{R}^n)}(h^{3(1-2\delta)}). \tag{4.20}$$

Remark 4.32. *Let a, b be symbols, then $\overline{a\#b} = \overline{b}\#\overline{a}$ and $\overline{a}\#a$ is real-valued.*

Proof. We have for all $z \in \mathbb{R}^{2n}$ that

$$\begin{aligned} \overline{a\#b}(z) &= \overline{e^{\frac{i}{2h}\sigma(hD_z, hD_w)}(a(z)b(w))}\Big|_{z=w} = e^{-\frac{i}{2h}\sigma(hD_z, hD_w)}(\overline{a(z)b(w)})\Big|_{z=w} \\ &= e^{\frac{i}{2h}\sigma(hD_w, hD_z)}(\overline{b(w)a(z)})\Big|_{z=w} = \overline{b}\#\overline{a}(z). \end{aligned}$$

Now let $a = b + ic$ where $b, c : \mathbb{R}^{2n} \to \mathbb{R}$. Then

$$\overline{a(z)}a(w) = b(z)b(w) + c(z)c(w) + i(b(z)c(w) - b(w)c(z)) =: A(z, w) + iB(z, w)$$

where $A(z, w) = A(w, z)$ and $B(z, w) = -B(w, z)$ for all $z, w \in \mathbb{R}^{2n}$. Then for all $k \in \mathbb{N}$,

$$\begin{aligned} \sigma(D_z, D_w)^{2k+1} A(z, w)\big|_{z=w} &= -\sigma(D_w, D_z)^{2k+1} A(w, z)\big|_{z=w} \\ \sigma(D_z, D_w)^{2k} B(z, w)\big|_{z=w} &= -\sigma(D_w, D_z)^{2k} B(w, z)\big|_{z=w}. \end{aligned}$$

Hence $\sigma(D_z, D_w)^{2k+1} A(z, w)|_{z=w} = \sigma(D_z, D_w)^{2k} B(z, w)|_{z=w} = 0$. From formula (4.18) it is clear that $\overline{a}\#a$ is indeed real-valued. $\square$

Next, we want to prove that $a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ for symbols $a \in S_\delta(m)$. This is true for all order functions m such that $\sup m < \infty$. We will prove this using the Cotlar-Stein theorem.

Theorem 4.33. *(Cotlar-Stein theorem) Let H_1, H_2 be Hilbert spaces and let $A_j : H_1 \to H_2$ be linear operators for all $j \in \mathbb{N}$. If there is a constant $C > 0$ such that*

$$\sup_{j \in \mathbb{N}} \sum_{k=1}^\infty \|A_j^* A_k\|^{\frac{1}{2}} \leq C, \qquad \sup_{j \in \mathbb{N}} \sum_{k=1}^\infty \|A_j A_k^*\|^{\frac{1}{2}} \leq C, \tag{4.21}$$

then $\sum_{j=1}^\infty A_j$ converges in the strong topology, i.e. $\sum_{j=1}^\infty A_j u \in H_2$ for all $u \in H_1$, and $\|\sum_{j=1}^\infty A_j\| \leq C$.

So our goal is to construct a sequence $\{A_j : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)\}_{j \in \mathbb{N}}$ that satisfies the conditions of the Cotlar-Stein theorem and converges to $a^W(x, hD)$. We will use the following contruction to cut the symbol $a \in S_\delta(m)$ into compactly supported symbols a_α for $\alpha \in \mathbb{Z}^{2n}$.

Let $\chi \in C_c^\infty(\mathbb{R}^{2n})$ such that $0 \leq \chi \leq 1$ and $\sum_{\alpha \in \mathbb{Z}^{2n}} \chi(z - \alpha) = 1$ for all $z \in \mathbb{R}^{2n}$. Such a function can be constructed as follows: define for $0 \leq j \leq 2n$, $\chi_j(z) := \frac{1}{2}\cos(\pi z_j) + \frac{1}{2}$ if $z_j \in [-1, 1]$, and $\chi_j(z) := 0$ otherwise. Then the function $\chi := \Pi_{j=1}^{2n} \chi_j$ satisfies the required properties.

Now define the function $a_\alpha \in \mathscr{S}(\mathbb{R}^{2n})$ for all $\alpha \in \mathbb{Z}^{2n}$ by $a_\alpha(z) := \chi(z-\alpha)a(z)$. Then $\sum_{\alpha\in\mathbb{Z}^{2n}} a_\alpha \equiv 1$. Now let $A_\alpha := a_\alpha^W(x, hD)$. Our goal is to show that there is a constant $C > 0$ such that

$$\begin{aligned}
C &\geq \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|A_j^* A_k\|^{\frac{1}{2}} = \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|a_\alpha^W(x,hD)^* a_\beta^W(x,hD)\|^{\frac{1}{2}} \\
&= \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|\overline{a}_\alpha^W(x,hD) a_\beta^W(x,hD)\|^{\frac{1}{2}} = \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|(\overline{a}_\alpha \# a_\beta)^W(x,hD)\|^{\frac{1}{2}}, \\
C &\geq \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|A_j A_k^*\|^{\frac{1}{2}} = \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|a_\alpha^W(x,hD) a_\beta^W(x,hD)^*\|^{\frac{1}{2}} \\
&= \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|a_\alpha^W(x,hD) \overline{a}_\beta^W(x,hD)\|^{\frac{1}{2}} = \sup_{\alpha\in\mathbb{Z}^{2n}} \sum_{\beta\in\mathbb{Z}^{2n}} \|(a_\alpha \# \overline{a}_\beta)^W(x,hD)\|^{\frac{1}{2}}.
\end{aligned}$$

The following lemma shows that $\overline{a}_\alpha \# a_\beta$ and its derivatives vanish rapidly if α and β or if z and $(\alpha+\beta)/2$ are far apart.

Lemma 4.34. *(Mixed term decay) Let $0 \leq \delta \leq 1/2$ and let m be a bounded order function. Let $a \in S_\delta(m)$ and define a_α as above. For all $\alpha, \beta \in \mathbb{Z}^{2n}$, $N \in \mathbb{N}$, and multi-indices $\gamma \in \mathbb{N}^{2n}$ there is a constant $C_{\gamma,N} > 0$, such that for all $z \in \mathbb{R}^{2n}$;*

$$|\partial^\gamma \overline{a}_\alpha \# a_\beta(z)| \leq C_{\gamma,N} \langle \alpha - \beta \rangle^{-N} \langle z - \frac{\alpha+\beta}{2} \rangle^{-N}. \tag{4.22}$$

Moreover, there is a constant $C_{\gamma,N} > 0$ not depending on a or h, and a $K \in \mathbb{N}$ depending linearly on n, such that for all $z \in \mathbb{R}^{2n}$;

$$|\partial^\gamma \overline{a}_\alpha \# a_\beta(z)| \leq C_{\gamma,N} \left(\sum_{|\kappa|\leq K} h^{|\kappa|/2} |\sup \partial^\kappa a| \right)^2 \langle \alpha - \beta \rangle^{-N} \langle z - \frac{\alpha+\beta}{2} \rangle^{-N}. \tag{4.23}$$

and there is a constant $C_{\gamma,N} > 0$ possibly depending on h, such that for all $z \in \mathbb{R}^{2n}$;

$$|\partial^\gamma \overline{a}_\alpha \# a_\beta(z)| \leq C_{\gamma,N} m(\alpha) m(\beta) \langle \alpha - \beta \rangle^{-N} \langle z - \frac{\alpha+\beta}{2} \rangle^{-N}. \tag{4.24}$$

Proof. Recall that

$$\begin{aligned}
\overline{a}_\alpha \# a_\beta(z) &= \frac{1}{(\pi h)^{2n}} \int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[e^{-\frac{2i}{h}\sigma(w_1,w_2)} \overline{a_\alpha(z+w_1)} a_\beta(z+w_2) \right] \\
&= \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} d\tilde{w}_1 \int_{\mathbb{R}^{2n}} d\tilde{w}_2 \left[e^{-2i\sigma(\tilde{w}_1,\tilde{w}_2)} \overline{a_\alpha(h^{1/2}(\tilde{z}+\tilde{w}_1))} a_\beta(h^{1/2}(\tilde{z}+\tilde{w}_2)) \right] \\
&= \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} d\tilde{w}_1 \int_{\mathbb{R}^{2n}} d\tilde{w}_2 \left[e^{-2i\sigma(\tilde{w}_1,\tilde{w}_2)} \overline{\tilde{a}_\alpha(\tilde{z}+\tilde{w}_1)} \tilde{a}_\beta(\tilde{z}+\tilde{w}_2) \right],
\end{aligned}$$

where we put $\tilde{w}_1 := h^{-1/2} w_1$, $\tilde{w}_2 := h^{-1/2} w_2$, $\tilde{z} := h^{-1/2} z$, and $\tilde{a}_\alpha(\tilde{z}) := a_\alpha(z) = a_\alpha(h^{1/2}\tilde{z})$. For the sake of readability, all tildes will be omitted for now. For any multi-index γ we have

$$\partial^\gamma \overline{a}_\alpha \# a_\beta(z) = \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[e^{-2i\sigma(w_1,w_2)} \partial_z^\gamma \left(\overline{a_\alpha(z+w_1)} a_\beta(z+w_2) \right) \right].$$

Note that the support of our choice of χ lies in $B(0,n)$, so the integrand is just zero unless $z + w_1 - \alpha, z + w_2 - \beta \in B(0,n)$. We obtain

$$\begin{aligned}
|\alpha - \beta| &= |(z - \beta + w_2) - (z - \alpha + w_1) - w_2 + w_1| \leq 2n + |w_1| + |w_2|, \\
\left| z - \frac{a+b}{2} \right| &= \frac{1}{2} |(z - \alpha + w_1) - w_1 + (z - \beta + w_2) - w_2| \leq 2n + |w_1| + |w_2|,
\end{aligned}$$

hence for some constant $C > 0$ such that $\langle \alpha - \beta \rangle \le C\langle w \rangle$ and $\langle z - (\alpha+\beta)/2 \rangle \le C\langle w \rangle$ where $w := (w_1, w_2)$. So for any $N \in \mathbb{N}$, $\langle w \rangle^{-2N} \le C\langle \alpha - \beta \rangle^{-N} \langle z - (\alpha+\beta)/2 \rangle^{-N}$ for some constant $C > 0$.

We will obtain a factor $\langle w \rangle^{-2N}$ by integrating by parts. As will be clear shortly, integration by parts is only possible if $w := (w_1, w_2)$ lies outside an open neighbourhood of 0. We will cut the integral in two parts: one in a bounded neighbourhood of 0, and one outside of it. Let $\zeta : \mathbb{R}^{4n} \to [0, 1]$ be a smooth function such that $\zeta \equiv 1$ on $B(0, 1)$ and $\mathrm{Supp}(\zeta) \subset B(0, 2)$. Define for each multi-index γ:

$$A_\gamma(z) := \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[e^{-2i\sigma(w_1,w_2)} \zeta(w_1, w_2) \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right],$$
$$B_\gamma(z) := \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[e^{-2i\sigma(w_1,w_2)} (1 - \zeta(w_1, w_2)) \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right],$$

so that $\partial^\gamma \overline{a}_\alpha \# a_\beta(z) = A_\gamma(z) + B_\gamma(z)$ for all $z \in \mathbb{R}^{2n}$.

(Proof of (4.22).) We will first estimate $|\partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2))|$, and then $|A_\gamma(z)|$ and $|B_\gamma(z)|$.

- Since $\sup m < \infty$, we have
$$\left| \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right| \le C \sum_{|\kappa| \le |\gamma|} \left| \partial_z^\kappa (\overline{a_\alpha(z + w_1)}) \right| \left| \partial_z^{\gamma-\kappa} (a_\beta(z + w_2)) \right|$$
$$\le C_\gamma \sum_{|\kappa| \le |\gamma|} (\sup m)^2 \le C_\gamma.$$

- Since the support of ζ is bounded, clearly there is some constant $C_{\gamma,0} > 0$ such that $|A_\gamma(z)| \le C_{\gamma,0}$ for all $z \in \mathbb{R}^{2n}$. Furthermore, due to $|w| \le 2$ we have $\langle w \rangle^{-2N} \ge \langle 2 \rangle^{-2N}$. So we can define for any $N \in \mathbb{N}$, $C_{\gamma,N} := \langle 2 \rangle^{2N} C_{\gamma,0}$, then
$$|A_\gamma(z)| \le C_{\gamma,0} = C_{\gamma,N} \langle 2 \rangle^{-2N} \le C_{\gamma,N} \langle w \rangle^{-2N} \le C_{\gamma,N} \langle \alpha - \beta \rangle^{-N} \langle z - \frac{\alpha + \beta}{2} \rangle^{-N}.$$

- Now for $B_\gamma(z)$: it is convenient to write $\varphi(w) := -2\sigma(w_1, w_2) = -2(x_2\xi_1 - x_1\xi_2)$. It's derivatives are $\partial_{x_1}\varphi(w) = 2\xi_2$, $\partial \xi_1 \varphi(w) = -2x_2$, $\partial_{x_2}\varphi(w) = -2\xi_1$, and $\partial_{\xi_2}\varphi(w) = 2x_1$, so $|\partial\varphi(w)| = 2|w|$. Then we can define the operator
$$L := \frac{\langle \partial\varphi, D_w \rangle}{|\partial\varphi|^2} = \frac{\langle \partial\varphi, D_w \rangle}{|w|^2}$$
and this operator satisfies $Le^{-2i\sigma(w_1,w_2)} = e^{-2i\sigma(w_1,w_2)}$. Now we can integrate $B_\gamma(z)$ by parts. Note that the integrand vanishes in $B(0, 1)$, so there are no problems with $w = 0$.

$$\begin{aligned} &B_\gamma(z) \\ &= \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{2n}} dw_1 \int_{\mathbb{R}^{2n}} dw_2 \left[L^{2N+4n+1} \left(e^{-2i\sigma(w_1,w_2)} \right) (1 - \zeta(w_1, w_2)) \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right] \\ &= \frac{1}{\pi^{2n}} \int_{\mathbb{R}^{4n}} dw \left[\frac{e^{-2i\sigma(w_1,w_2)}}{|w|^{4N+8n+2}} (-\langle \partial\varphi, D_w \rangle)^{2N+4n+1} \left((1 - \zeta(w_1, w_2)) \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right) \right], \\ &|B_\gamma(z)| \le C_{\gamma,N} \int_{\mathbb{R}^{4n}} dw \left[\langle w \rangle^{-(2N+4n+1)} \right] \le C_{\gamma,N} \langle \alpha - \beta \rangle^{-N} \langle z - \frac{\alpha + \beta}{2} \rangle^{-N}. \end{aligned}$$

(Proof of (4.23).)

- Recall that for any two positive real numbers a and b, $ab \le \frac{1}{2}(a^2 + b^2)$ and $a^2 + b^2 \le (a + b)^2$. So we obtain
$$\left| \partial_z^\gamma (\overline{a_\alpha(z + w_1)} a_\beta(z + w_2)) \right| \le C \sum_{|\kappa| \le |\gamma|} \left| \partial_z^\kappa (\overline{a_\alpha(z + w_1)}) \right| \left| \partial_z^{\gamma-\kappa} (a_\beta(z + w_2)) \right|$$
$$\le C_\gamma \left(\sum_{|\kappa| \le |\gamma|} |\sup \partial^\kappa a| \right)^2.$$

- The rest of the proof is analogous to the previous proof. Putting the tildes back in, we obtain $\partial_{\tilde{z}}^{\kappa}\tilde{a}(\tilde{z}) = \partial_{\tilde{z}}^{\kappa}a(h^{1/2}\tilde{z}) = h^{|\kappa|/2}\partial_z^{\kappa}a(z)$, hence $|\sup \partial^{\kappa}\tilde{a}| = h^{|\kappa|/2}|\sup \partial^{\kappa}a|$.

(Proof of (4.24).)

- Note that m is an order function, so for some $M \in \mathbb{N}$, we have $m(w) \leq C\langle z - w\rangle^M m(z)$ for all $w, z \in \mathbb{R}^{2n}$. Then we obtain

$$\begin{aligned}|\partial_z^{\gamma}a_{\alpha}(w_1+z)| &= |\partial_z^{\gamma}(\chi(w_1+z-\alpha)a(w_1+z))| \leq C \sup_{|\kappa|\leq|\gamma|}|\partial_z^{\kappa}\chi(w_1+z-\alpha)|m(w_1+z)\\ &\leq C \sup_{|\kappa|\leq|\gamma|}|\partial_z^{\kappa}\chi(w_1+z-\alpha)|\langle w_1+z-\alpha\rangle^M m(\alpha) \leq C_{\gamma}m(\alpha),\end{aligned}$$

where we used that $|w_1 + z - \alpha| \leq n$. Hence $|\partial_z^{\gamma}(\overline{a_{\alpha}(z+w_1)}a_{\beta}(z+w_2))| \leq Cm(\alpha)m(\beta)$.

- The rest of the proof is again analogous to the first proof. ◻

Lemma 4.35. *(More on mixed term decay) For sufficiently large $N \in \mathbb{N}$, there is a constant $C_N > 0$ such that*

$$\|(\overline{a}_{\alpha}\#a_{\beta})^W(x,hD)\| \leq C_N\langle\alpha-\beta\rangle^{-N}. \tag{4.25}$$

Moreover, there is a constant $C_N > 0$ not depending on a or h, and a $K \in \mathbb{N}$ depending linearly on n, such that

$$\|(\overline{a}_{\alpha}\#a_{\beta})^W(x,hD)\| \leq C_N\left(\sum_{|\kappa|\leq K} h^{|\kappa|/2}|\sup \partial^{\kappa}a|\right)^2\langle\alpha-\beta\rangle^{-N}, \tag{4.26}$$

and there is a constant $C_N > 0$ possibly depending on h, such that

$$\|(\overline{a}_{\alpha}\#a_{\beta})^W(x,hD)\| \leq C_N m(\alpha)m(\beta)\langle\alpha-\beta\rangle^{-N}. \tag{4.27}$$

Proof. Recall that for any $a \in \mathscr{S}(\mathbb{R}^{2n})$, we have

$$a^W(x,hD) = \frac{1}{(2\pi h)^{2n}}\int_{\mathbb{R}^{2n}} dl\left[\hat{a}_h(l)e^{\frac{i}{h}l(x,hD)}\right].$$

Using lemma 3.6, we obtain

$$\begin{aligned}\|(\overline{a}_{\alpha}\#a_{\beta})^W(x,hD)\|_{L^2(\mathbb{R}^n)\to L^2(\mathbb{R}^n)} &\leq C\int_{\mathbb{R}^{2n}} dl\left[|\mathscr{F}_h(\overline{a}_{\alpha}\#a_{\beta})|\right] = C\|\mathscr{F}_h(\overline{a}_{\alpha}\#a_{\beta})\|_{L^1(\mathbb{R}^{2n})}\\ &\leq C\max_{|\gamma|\leq 2n+1}\|\partial^{\gamma}\overline{a}_{\alpha}\#a_{\beta}\|_{L^1(\mathbb{R}^{2n})}\\ &= C\max_{|\gamma|\leq 2n+1}\int_{\mathbb{R}^{2n}} dz\left[\partial^{\gamma}\overline{a}_{\alpha}\#a_{\beta}(z)\langle z\rangle^{2n+1}\langle z\rangle^{-(2n+1)}\right]\\ &\leq C\sup_{z\in\mathbb{R}^{2n}}\max_{|\gamma|\leq 2n+1}\langle z\rangle^{2n+1}\partial^{\gamma}\overline{a}_{\alpha}\#a_{\beta}(z)\\ &\leq C_N\sup_{z\in\mathbb{R}^{2n}}\langle z\rangle^{2n+1}\langle z-\frac{\alpha+\beta}{2}\rangle^{-N}\langle\alpha-\beta\rangle^{-N}\end{aligned}$$

for all $N \in \mathbb{N}$ according to (4.22) in the previous lemma. If N is sufficiently large, this supremum is finite and we obtain

$$\|(\overline{a}_{\alpha}\#a_{\beta})^W(x,hD)\|_{L^2(\mathbb{R}^n)\to L^2(\mathbb{R}^n)} \leq C_N\langle\alpha-\beta\rangle^{-N},$$

proving (4.25). Finally, (4.26) and (4.27) follow similarly from (4.23) and (4.24), respectively. ◻

Theorem 4.36. *Let m be a bounded order function and let $0 \leq \delta \leq 1/2$. Let $a \in S_\delta(m)$, then*

$$a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n), \tag{4.28}$$

and we can estimate its norm by

$$\|a^W(x, hD)\| \leq C \sum_{|\kappa| \leq K} h^{|\kappa|/2} \sup |\partial^\kappa a| \tag{4.29}$$

where $C > 0$, and $K \in \mathbb{N}$ does not depends on a and depends linearly on the dimension n.

Proof. By the previous lemma we have $\|(\overline{a}_\alpha \# a_\beta)^W(x, hD)\| \leq C_N \langle \alpha - \beta \rangle^{-N}$ for all $\alpha, \beta \in \mathbb{Z}^{2n}$ if $N \in \mathbb{N}$ is sufficiently large. Then

$$\sup_{\alpha \in \mathbb{Z}^{2n}} \sum_{\beta \in \mathbb{Z}^{2n}} \|(\overline{a}_\alpha \# a_\beta)^W(x, hD)\|^{1/2} \leq C_N \sup_{\alpha \in \mathbb{Z}^{2n}} \sum_{\beta \in \mathbb{Z}^{2n}} \langle \alpha - \beta \rangle^{-N/2} = C_N \sum_{\beta \in \mathbb{Z}^{2n}} \langle \beta \rangle^{-N/2} < \infty$$

if N is large enough. Similarly, $\sup_{\alpha \in \mathbb{Z}^{2n}} \sum_{\beta \in \mathbb{Z}^{2n}} \|(a_\alpha \# \overline{a}_\beta)^W(x, hD)\|^{1/2}$ is finite as well. Now by the Cotlar-Stein theorem, $\sum_{\alpha \in \mathbb{Z}^{2n}} a_\alpha^W(x, hD)$ converges in the strong topology. And $a^W(x, hD) = \sum_\alpha a_\alpha^W(x, hD)$ due to $a = \sum_\alpha a_\alpha$.

The estimate follows immediately from (4.26). □

Theorem 4.37. *Let $0 \leq \delta \leq 1/2$ and let m be an order function such that $\lim_{z \to \infty} m(z) = 0$. Let $a \in S_\delta(m)$, then $a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is a compact operator.*

Proof. Note that each a_α is a Schwartz function, so $a_\alpha^W(x, hD)$ is a compact operator for all $\alpha \in \mathbb{Z}^{2n}$. Let $0 < M_1 < M_2$. The compact operators are closed in the norm topology, so it suffices to show that $\sum_{|\alpha| < M_1} a_\alpha^W(x, hD)$ converges in norm to $a^W(x, hD)$ as $M_1 \to \infty$. Consider

$$\sum_{\alpha < M_2} a_\alpha^W(x, hD) - \sum_{|\alpha| < M_1} a_\alpha^W(x, hD) = \sum_{M_1 \leq |\alpha| < M_2} a_\alpha^W(x, hD),$$

and note that there is some $M > 0$ such that $m(\beta) \leq C\langle \alpha - \beta \rangle^M m(\alpha)$ because m is an order function. Now we can use (4.27) to obtain for sufficiently large N that

$$\begin{aligned}
\sup_{|\alpha| > M_1} \sum_{\beta > M_1} \|(\overline{a}_\alpha \# a_\beta)^W(x, hD)\|^{1/2} &\leq C_N \sup_{|\alpha| > M_1} \sum_{\beta > M_1} \sqrt{m(\alpha) m(\beta)} \langle \alpha - \beta \rangle^{-N/2} \\
&\leq C_N \sup_{|\alpha| > M_1} m(\alpha) \sum_{\beta > M_1} \langle \alpha - \beta \rangle^{(M-N)/2} \\
&= C \sup_{|\alpha| > M_1} m(\alpha)
\end{aligned}$$

if N is sufficiently large. Analogously, we obtain the same estimate for $a_\alpha \# \overline{a}_\beta$. By the Cotlar-Stein theorem, $\sum_{M_1 < |\alpha| < M_2} a_\alpha^W(x, hD)$ converges in the strong topology to $\sum_{|\alpha| > M_1} a_\alpha^W(x, hD)$ and it satisfies $\| \sum_{|\alpha| > M_1} a_\alpha^W(x, hD)\| \leq C \sup_{|\alpha| > M_1} m(\alpha)$. This indeed converges to 0 as $M_1 \to \infty$. □

4.4 Computing the quantisation of various symbols

We will now compute $a^W(x, hD)$ for various symbols. Recall that $m_{k,l}(x, \xi) := \langle x \rangle^k + \langle \xi \rangle^l$, where $k, l \in \mathbb{R}$.

Lemma 4.38. *(Symbols depending only on x) Let $a \in S_\delta(m_{k,0})$ such that a does not depend on ξ, then $Op_t(a)u(x) = a(x)u(x)$ for all $t \in [0, 1]$.*

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$, then

$$a(x, hD)u(x) = \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x - y, \xi \rangle} a(x) u(y) \right] = a(x)u(x).$$

But we also have

$$\begin{aligned}
\partial_t Op_t(a)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\partial_t a(tx+(1-t)y)u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\sum_{j=1}^n(\partial_j a)(tx+(1-t)y)(x_j-y_j)u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \int_{\mathbb{R}^n} dy \left[\sum_{j=1}^n hD_{\xi_j}e^{\frac{i}{h}\langle x-y,\xi\rangle}(\partial_j a)(tx+(1-t)y)u(y)\right] \\
&= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi \left[\frac{h}{i}\nabla_\xi e^{\frac{i}{h}\langle x,\xi\rangle}\hat{b}_h(\xi)\right]
\end{aligned}$$

where $b:\mathbb{R}^n\to\mathbb{C}^n, y\mapsto \partial a(x+(1-t)y)u(y)$. Note that $b_j\in\mathscr{S}(\mathbb{R}^n)$ for all $1\le j\le n$, so $\mathscr{F}_h(b_j)\in\mathscr{S}(\mathbb{R}^n)$ and so $\hat{b}_h(\xi)\to 0$ as $|\xi|\to\infty$. So $\partial_t Op_t(a)u(x)=0$ for all $t\in[0,1]$, hence

$$Op_t(a)u(x) = a(x,hD)u(x) = a(x)u(x)$$

as desired. □

Lemma 4.39. *(Symbols depending linearly on ξ) Let $a(x,\xi)=\langle c(x),\xi\rangle_{\mathbb{R}^n}$ for some continuously differentiable map $c:\mathbb{R}^n\to\mathbb{C}^n$, then*

$$\begin{aligned}
a^W(x,hD)u &= \frac{1}{2}\sum_{j=1}^n\left(hD_{x_j}(c_j u)+c_j hD_{x_j}(u)\right) && (4.30)\\
&= \frac{h}{i}\sum_{j=1}^n\left[\frac{1}{2}\partial_j(c_j)u + c_j\partial_j u\right]. && (4.31)
\end{aligned}$$

Proof. We have $a(x,\xi)=\sum_{j=1}^n c_j(x)\xi_j$, so for all $u\in\mathscr{S}(\mathbb{R}^n)$,

$$\begin{aligned}
a^W(x,hD)u(x) &= \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi\int_{\mathbb{R}^n} dy\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\sum_{j=1}^n c_j\left(\frac{x+y}{2}\right)\xi_j u(y)\right] \\
&= \sum_{j=1}^n \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi\int_{\mathbb{R}^n} dy\left[-hD_{y_j}\left(e^{\frac{i}{h}\langle x-y,\xi\rangle}\right)c_j\left(\frac{x+y}{2}\right)u(y)\right] \\
&= \sum_{j=1}^n \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi\int_{\mathbb{R}^n} dy\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}hD_{y_j}\left(c_j\left(\frac{x+y}{2}\right)u(y)\right)\right] \\
&= \sum_{j=1}^n \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^n} d\xi\int_{\mathbb{R}^n} dy\left[e^{\frac{i}{h}\langle x-y,\xi\rangle}\left(\frac{1}{2}(hD_{x_j}c_j)\left(\frac{x+y}{2}\right)u(y)+c_j\left(\frac{x+y}{2}\right)(hD_{x_j}u)(y)\right)\right] \\
&= \sum_{j=1}^n\left[\left(\frac{1}{2}hD_{x_j}c_j\right)^W(x,hD)u(x)+c_j^W(x,hD)(hD_{x_j}u)(x)\right] \\
&= \sum_{j=1}^n\left[\left(\frac{1}{2}hD_{x_j}c_j\right)(x)u(x)+c_j(x)(hD_{x_j}u)(x)\right] \\
&= \frac{h}{i}\sum_{j=1}^n\left[\frac{1}{2}\partial_j(c_j)(x)u(x)+c_j(x)\partial_j u(x)\right].
\end{aligned}$$

□

Lemma 4.40. *(Symbols depending quadratically on ξ) Let $a(x,\xi) = \sum_{i,j=1}^n c^{ij}(x)\xi_i\xi_j$, then*

$$a^W(x,hD)u = \frac{1}{4}\sum_{i,j=1}^n \big(hD_{x_i}hD_{x_j}(c^{ij}u) + hD_{x_i}(c^{ij}hD_{x_j}u) + hD_{x_j}(c^{ij}hD_{x_i}u) + c^{ij}hD_{x_i}hD_{x_j}u\big) \quad (4.32)$$

$$= -h^2\sum_{i,j=1}^n \left[\frac{1}{4}\partial_i\partial_j(c^{ij})u + \frac{1}{2}\partial_i c^{ij}\partial_j u + \frac{1}{2}\partial_j c^{ij}\partial_i u + c^{ij}\partial_i\partial_j u\right] \quad (4.33)$$

Proof. The proof is very similar to the previous proof and will be omitted. □

In particular, if $p(x,\xi) = |\xi|^2 + V(x)$, then $p^W(x,hD) := -h^2\sum_{i=1}^n \partial_{x_i}^2 + V(x) = -h^2\Delta + V(x)$.

5 Tunneling

In classical physics, the total energy of a system is given by $p(x,\xi) := |\xi|^2 + V(x)$, the sum of kinetic energy and potential energy. Let $E \in \mathbb{R}$ be some energy level, i.e. $p(x,\xi) = E$. Since the kinetic energy $|\xi|^2$ is nonnegative, it follows that the domain

$$\{x \in \mathbb{R}^n \mid V(x) > E\}$$

is not available to such a system. As a result, the connected components of $\{x \in \mathbb{R}^n \mid V(x) \le E\}$ are separated from one another by a 'hard' potential barrier that cannot be crossed.

The goal of this section is to explore the behaviour of an eigenfunction u of the Schrödinger operator

$$P(h) := p^W(x, hD) = -h^2\Delta + V$$

with eigenvalue E on the classically forbidden domain $\{x \in \mathbb{R}^n \mid V(x) > E\}$ in the semiclassical limit $h \to 0$. We will find for any $U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > 0\}$ that there are constants $0 < \delta < \gamma$ such that

$$e^{-\gamma/h} \le \|u\|_{L^2(U)} \le e^{-\delta/h}$$

as $h \to 0$. These two inequalities are called the Carleman inequality and the Agmon-Lithner estimate, respectively. As a result, the wave function u is exponentially small on the classical forbidden domain as $h \to 0$, but it does not vanish. This stands in stark contrast with the classical case, since the connected components of $\{x \in \mathbb{R}^n \mid V(x) \le E\}$ are only separated by a 'soft' barrier that can be 'tunneled' through.

Even though $P(h)$ is not a bounded operator $L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, it will still prove useful to prepare a few results on symbols in S.

5.1 Gårding inequality

In this subsection, we will study real-valued symbols in greater detail and prove the Gårding inequality. First, we need a useful lemma that proves that the operator $a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is invertible under certain conditions on the symbol a.

Definition 5.1. *(Elliptic symbols) A symbol $a \in S_\delta(m)$ is called elliptic if $|a| \ge \gamma m$ for some constant $\gamma > 0$ that does not depend on h.*

Proposition 5.2. *(Elliptic symbols give rise to invertible operators) Let $0 \le \delta < \frac{1}{2}$, let m be an order function such that $\inf_{z,h} m(z) > 0$, and let $a \in S_\delta(m)$ be elliptic. Then there exist $h_0, C > 0$ such that*

$$\|a^W(x, hD)u\|_{L^2} \ge C\|u\|_{L^2} \tag{5.1}$$

for all $u \in \mathscr{S}(\mathbb{R}^n)$ and all $0 < h \le h_0$.

If, in addition, $\sup_{z,h} m(z) < \infty$, then there is a constant $h_0 > 0$ such that $a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is invertible as a bounded linear operator on $L^2(\mathbb{R}^n)$ for all $0 < h \le h_0$.

Remark 5.3. *The condition that $\inf_{z,h} m(z) > 0$ and $\sup_{z,h} < \infty$ implies that $S_\delta(m) = S_\delta$.*

Proof. Since a is elliptic and $\inf m(z) > 0$, we have $\inf |a(z)| > 0$ and so $a^{-1} : \mathbb{R}^n \to \mathbb{C}, z \mapsto 1/a(z)$ is well-defined. We have $a \in S_\delta(m)$, i.e. for all multi-indices α, $|\partial^\alpha a| \le C_\alpha h^{-\delta|\alpha|} m$. Moreover, since a is elliptic, there is some constant $C > 0$ such that $\frac{1}{a} \le C\frac{1}{m}$. It is easy to verify that for any multi-index α, there is some constant $C_\alpha > 0$ such that $|\partial^\alpha \frac{1}{a}| \le C_\alpha h^{-\delta|\alpha|}\frac{1}{m}$, hence $1/a \in S_\delta(1/m)$.

By proposition 4.30 we obtain

$$a\#a^{-1} = 1 + O_{S_\delta}(h^{1-2\delta}),$$
$$a^{-1}\#a = 1 + O_{S_\delta}(h^{1-2\delta}).$$

Let $r_1, r_2 \in h^{1-2\delta}S_\delta$ such that $a\#a^{-1} = 1 + r_1$ and $a^{-1}\#a = 1 + r_2$, then by theorem 4.36 we have $(a^{-1})^W(x, hD), r_1^W(x, hD), r_2^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$. Furthermore, we have

$$a^W(x, hD)(a^{-1})^W(x, hD) = I + r_1^W(x, hD)$$

and

$$(a^{-1})^W(x, hD)a^W(x, hD) = I + r_2^W(x, hD)$$

where $\|r_1^W(x, hD)\|, \|r_2^W(x, hD)\| = O(h^{1-2\delta})$. Let $h_0 > 0$ be small enough so that $\|r_2^W(x, hD)\| < 1$ for all $0 < h \leq h_0$, then $I + r_2^W(x, hD)$ is invertible by lemma C.4. Hence for all $u \in L^2(\mathbb{R}^n)$,

$$\|u\| = \|(I + r_2^W(x, hD))^{-1}(a^{-1})^W(x, hD)a^W(x, hD)u\| \leq C\|a^W(x, hD)u\|.$$

Now assume that $\sup m(z) < \infty$. Note that in this case, $S_\delta(m) = S_\delta(1/m) = S_\delta$. Now, we also have $a^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$. Let $h_0 > 0$ be small enough such that $\|r_1^W(x, hD)\| < 1$ as well as $\|r_2^W(x, hD)\| < 1$, then $(a^{-1})^W(x, hD)$ is an approximate inverse for $a^W(x, hD)$ and so $a^W(x, hD)$ is invertible by proposition C.5. □

Lemma 5.4. *(Weak Gårding inequality) Let $a \in S$ be real-valued, define $a_\wedge := \inf a$, and let $\epsilon > 0$, then there is a $h_0 > 0$ such that for all $0 < h \leq h_0$ and all $u \in L^2(\mathbb{R}^n)$, we have*

$$\langle u, a^W(x, hD)u\rangle \geq (a_\wedge - \epsilon)\|u\|^2. \tag{5.2}$$

Proof. Let $\lambda \leq a_\wedge - \epsilon$, then $a - \lambda \geq \epsilon > 0$ and so $a - \lambda$ is elliptic. So there is a $h_0(\lambda) > 0$ such that $a^W(x, hD) - \lambda I$ is invertible for all $0 < h \leq h_0(\lambda)$. We want to show that we can in fact pick $h_0 > 0$ independent of λ.

As in the proof of the previous lemma, we can write

$$(a - \lambda)\#(a - \lambda)^{-1} = 1 + r_1(\lambda),$$
$$(a - \lambda)^{-1}\#(a - \lambda) = 1 + r_2(\lambda),$$

where $r_1(\lambda), r_2(\lambda) \in hS$. Since $r_1(\lambda)$ and $r_2(\lambda)$ are given by formula (4.18), it is clear they only depend on powers of derivatives of a and on powers of $(a - \lambda)^{-1}$. Hence we have for all $\lambda \leq a_\wedge - \epsilon$ that $r_1(\lambda) \leq r_1(a_\wedge - \epsilon)$ and $r_2(\lambda) \leq r_2(a_\wedge - \epsilon)$.

Now let $h_0 := h_0(a_\wedge - \epsilon) > 0$, then for all $\lambda \leq a_\wedge - \epsilon$ and all $0 < h \leq h_0$, the operator $a^W(x, hD) - \lambda I$ is invertible. Hence $\sigma(a^W(x, hD)) \subset [a_\wedge - \epsilon, \infty)$. So, by proposition C.9, we obtain

$$\langle u, a^W(x, hD)u\rangle \geq (a_\wedge - \epsilon)\|u\|^2$$

for all $u \in L^2(\mathbb{R}^n)$. □

Theorem 5.5. *(Gårding inequality) Let $a \in S$ be real-valued, define $a_\wedge := \inf a$. Then there is a sufficiently small constant $h_0 > 0$ and a sufficiently large constant $\gamma > 0$ such that for all $0 < h \leq h_0$ and all $u \in L^2(\mathbb{R}^n)$, we have*

$$\langle u, a^W(x, hD)u\rangle \geq (a_\wedge - h\gamma)\|u\|^2. \tag{5.3}$$

Proof. Let $\gamma > 0$ and let $\lambda \leq a_\wedge - h\gamma$. Then $a - \lambda \geq h\gamma > 0$. Note that this does not imply that $a - \lambda$ is elliptic since the lower bound $h\gamma$ depends on h. But $(a - \lambda)^{-1}$ is well-defined still. Recall that

$$(a - \lambda)\#(a - \lambda)^{-1} = e^{\frac{i}{2h}\sigma(hD_z, hD_w)}\left((a(z) - \lambda)(a(w) - \lambda)^{-1}\right)|_{z=w}.$$

Now we can define $f(t) := e^{\frac{it}{2h}\sigma(hD_z, hD_w)}\left((a(z) - \lambda)(a(w) - \lambda)^{-1}\right)|_{z=w}$ and apply Taylor's theorem around $t = 0$ to obtain

$$\begin{aligned}
&(a - \lambda)\#(a - \lambda)^{-1} \\
&\quad = 1 + \int_0^1 dt\left[(1 - t)e^{\frac{it}{2h}\sigma(hD_z, hD_w)}\left(\frac{i}{2h}\sigma(hD_z, hD_w)\right)^2\left((a(z) - \lambda)(a(w) - \lambda)^{-1}\right)|_{z=w}\right] \\
&\quad =: 1 + r_\lambda(z),
\end{aligned}$$

where we used that $f(1) = (a-\lambda)\#(a-\lambda)^{-1}$, $f(0) = 1$, and $\partial_t f(0) = 0$. Assume for the moment that $h\gamma(a - a_\wedge + h\gamma)^{-1} \in S_{\frac{1}{2}}$ for all $0 < h \le h_0(\gamma)$ for some sufficiently small $h_0(\gamma) > 0$ and sufficiently large $\gamma > 0$. Here we assume that the bounds do not depend on h or γ, i.e. $|\partial^\alpha h\gamma(a-a_\wedge+h\gamma)^{-1}| \le C_\alpha h^{-|\alpha|/2}$ for all multi-indices α and constants $C_\alpha > 0$ not depending on h or γ.

Then we have for multi-indices α s.t. $|\alpha| = 2$ that $h^2\gamma\partial^\alpha(a - a_\wedge + h\gamma)^{-1} \in S_{\frac{1}{2}}$, hence $\gamma r_{a_\wedge - h\gamma} \in S_{\frac{1}{2}}$ due to $a \in S \subset S_{\frac{1}{2}}$ and $e^{\frac{it}{2h}\sigma(hD_z, hD_w)} : S_\delta \to S_\delta$. But $|\partial^\alpha r_\lambda| \le |\partial^\alpha r_{a_\wedge - h\gamma}|$ for all multi-indices α, so for all $\lambda \le a_\wedge - h\gamma$ we have $\gamma r_\lambda \in S_{\frac{1}{2}}$. Hence $r_\lambda^W(x, hD) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ and

$$\|r_\lambda^W(x, hD)\| \le \|r_{a_\wedge - h\gamma}^W(x, hD)\| \le C/\gamma,$$

where $C > 0$ does not depend on γ. Note that C also does not depend on h due to $\delta = 1/2$.

Now if γ is sufficiently large, we obtain $\|r_\lambda^W(x, hD)\| < 1$. We can obtain a similar estimate for $(a-\lambda)^{-1}\#(a-\lambda)$, so $a^W(x, hD) - \lambda I$ is invertible for all $\lambda \le a_\wedge - h\gamma$. So $\sigma(a^W(x, hD)) \subset [a_\wedge - h\gamma, \infty)$ and hence $\langle u, a^W(x, hD)u\rangle \ge (a_\wedge - h\gamma)\|u\|^2$ for all $u \in L^2(\mathbb{R}^n)$.

It is only left to show that $h\gamma(a - a_\wedge + h\gamma)^{-1} \in S_{\frac{1}{2}}$ is indeed true. Let α be a multi-index, then

$$\partial^\alpha(a - a_\wedge + h\gamma)^{-1} = (a - a_\wedge + h\gamma)^{-1} \sum_{k=1}^{|\alpha|} \sum_{\substack{\alpha=\beta_1+\cdots+\beta_k, \\ |\beta_j|\ge 1}} C_{\beta_1,\cdots,\beta_k} \prod_{j=1}^{k} \left((a - a_\wedge + h\gamma)^{-1}\partial^{\beta_j} a\right),$$

for certain constants $C_{\beta_1,\cdots,\beta_k} \in \mathbb{R}$ for each partition of α. This is easy to show by induction to $|\alpha|$ and the product rule and chain rule. Since $a \in S$, we have for all multi-indices β that $|\partial^\beta a| \le C_\beta$. We can apply inequality B.3 to obtain $|\partial_j a| \le C(a - a_\wedge)^{1/2}$ for all $1 \le j \le n$. But then

$$\begin{aligned}(a - a_\wedge + h\gamma)^{-1}|\partial_j a| &\le C(a - a_\wedge + h\gamma)^{-1}(a - a_\wedge)^{1/2}(h\gamma)^{1/2}(h\gamma)^{-1/2} \\ &\le C(a - a_\wedge + h\gamma)^{-1}(a - a_\wedge + h\gamma)(h\gamma)^{-1/2} \\ &= C(h\gamma)^{-1/2},\end{aligned}$$

where we used the Cauchy-Schwarz inequality. For higher order derivatives $|\beta| \ge 2$ we simply have $(a - a_\wedge + h\gamma)^{-1}|\partial^\beta a| \le C_\beta(a - a_\wedge + h\gamma)^{-1} \le C_\beta(h\gamma)^{-1}$. Assume $h_0(\gamma) > 0$ is small enough so that $h_0\gamma \le 1$, then for all $0 < h \le h_0$ and all multi-indices $|\beta| \ge 1$, $(a - a_\wedge + h\gamma)|\partial^\beta a| \le C(h\gamma)^{-|\beta|/2}$. Finally, we obtain for all multi-indices α that

$$|\partial^\alpha(a - a_\wedge + h\gamma)^{-1}| \le C_\alpha(a - a_\wedge + h\gamma)^{-1}(h\gamma)^{-|\alpha|/2} \le C_\alpha(h\gamma)^{-1}h^{-|\alpha|/2}.$$

Hence $h\gamma|\partial^\alpha(a - a_\wedge + h\gamma)^{-1}| \le C_\alpha h^{-|\alpha|/2}$ for all $0 < h \le h(\gamma)$ as desired. □

5.2 Agmon-Lithner inequality

We will now consider the Schrödinger operator $P(h) := -h^2\Delta + V$ where $V : \mathbb{R}^n \to \mathbb{R}$ is a potential function not depending on h. The symbol associated with this operator is $p(x, \xi) := |\xi|^2 + V(x)$, the sum of the kinetic and the potential energy. Consider the eigenvalue equation

$$P(h)u = E(h)u \tag{5.4}$$

where $E(h) \in \mathbb{R}$. In this subsection, we want to prove that for each $U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > E\}$ there is some sufficiently small $\delta > 0$ such that $\|u\|_{L^2(U)} \le e^{-\delta/h}$ as $h \to 0$.

It will be convenient to consider the operator $P_\varphi(h)u := e^{\varphi/h}P(h)\left(e^{-\varphi/h}u\right)$ for some smooth function $\varphi : \mathbb{R}^n \to \mathbb{C}$. Assume for the moment that $u \in \mathscr{S}(\mathbb{R}^n)$, then

- $$\begin{aligned}\Delta(\varphi u) &= \sum_{j=1}^n \partial_j^2(\varphi u) = \sum_{j=1}^n \partial_j((\partial_j\varphi)u + \varphi(\partial_j u)) = \sum_{j-1}^n((\partial_j^2\varphi)u + 2(\partial_j\varphi)(\partial_j u) + \varphi(\partial_j^2 u))\\ &= (\Delta\varphi)u + 2\langle\partial\varphi, \partial u\rangle_{\mathbb{R}^n} + \varphi\Delta u,\end{aligned}$$
- $$\begin{aligned}\Delta e^{-\varphi/h} &= \sum_{j=1}^n \partial_j^2 e^{-\varphi/h} = \sum_{j=1}^n \partial_j\left(-\frac{1}{h}e^{-\varphi/h}\partial_j\varphi\right) = \sum_{j=1}^n\left(\frac{1}{h^2}e^{-\varphi/h}(\partial_j\varphi)^2 - \frac{1}{h}e^{-\varphi/h}\partial_j^2\varphi\right)\\ &= \frac{1}{h^2}e^{-\varphi/h}|\partial\varphi|^2 - \frac{1}{h}e^{-\varphi/h}\Delta\varphi,\end{aligned}$$
- $$\begin{aligned}\Delta\left(e^{-\varphi/h}u\right) &= \left(\Delta e^{-\varphi/h}\right)u + 2\langle\partial e^{-\varphi/h}, \partial u\rangle_{\mathbb{R}^n} + e^{-\varphi/h}\Delta u\\ &= \frac{1}{h^2}e^{-\varphi/h}|\partial\varphi|^2 u - \frac{1}{h}e^{-\varphi/h}(\Delta\varphi)u - \frac{2}{h}e^{-\varphi/h}\langle\partial\varphi, \partial u\rangle_{\mathbb{R}^n} + e^{-\varphi/h}\Delta u,\end{aligned}$$
- $$P_\varphi(h)u = -|\partial\varphi|^2 u + h(\Delta\varphi)u + 2h\langle\partial\varphi, \partial u\rangle_{\mathbb{R}^n} - h^2\Delta u + Vu.$$

Now define $p_\varphi : \mathbb{R}^n \to \mathbb{C}$ by

$$\begin{aligned}p_\varphi(x,\xi) &:= \langle\xi + i\partial\varphi(x), \xi + i\partial\varphi(x)\rangle_{\mathbb{R}^n} + V(x)\\ &= |\xi|^2 + 2i\langle\partial\varphi(x), \xi\rangle_{\mathbb{R}^n} - |\partial\varphi(x)|^2 + V(x).\end{aligned}$$

Let $u \in \mathscr{S}(\mathbb{R}^n)$, then we obtain for $p^W(x, hD)$ that

$$\begin{aligned}p^W(x,hD)u(x) &= -h^2\Delta u(x) + 2h\sum_{j=1}^n\left[\frac{1}{2}\partial_j^2\varphi(x)u(x) + \partial_j\varphi(x)\partial_j u(x)\right] - |\partial\varphi(x)|^2u(x) + V(x)u(x)\\ &= -h^2\Delta u(x) + h\Delta\varphi(x)u(x) + 2h\langle\partial\varphi(x), \partial u(x)\rangle_{\mathbb{R}^n} - |\partial\varphi(x)|^2u(x) + V(x)u(x)\\ &= P_\varphi(h)u(x).\end{aligned}$$

Hence $P_\varphi(h) = p_\varphi^W(x, hD)$ as operators $\mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$. Now we want to do the same for $u \in \mathscr{S}'(\mathbb{R}^n)$.

Lemma 5.6. *(Conjugation by φ) Let $\varphi : \mathbb{R}^n \to \mathbb{C}$ be smooth and define the symbol p_φ by*

$$p_\varphi(x,\xi) := \langle\xi + i\partial\varphi(x), \xi + i\partial\varphi(x)\rangle_{\mathbb{R}^n} + V(x).$$

Then we have for all $u \in \mathscr{S}'(\mathbb{R}^n)$ that

$$p_\varphi^W(x,hD)u(x) = e^{\varphi(x)/h}P(h)\left(e^{-\varphi/h}u\right)(x) =: P_\varphi u(x).$$

We need one more proposition before we can estimate $\|u\|_{L^2(U)}$. Consider the second order differential operator of the form $Q(h)u := -h^2\Delta u + \langle a, hDu\rangle + bu$ where $a, b : \mathbb{R}^n \to \mathbb{C}$. Then we can estimate the semiclassical Sobolev norm $\|u\|_{H_h^2(U)}$.

Proposition 5.7. *(H_h^2 estimate) Let $a, b : \mathbb{R}^n \to \mathbb{C}$ be smooth, define $Q(h)$ by*

$$Q(h)u := -h^2\Delta u + \langle a, hDu\rangle + bu$$

for all $u \in \mathscr{S}(\mathbb{R}^n)$. Let $U \subset\subset W \subset \mathbb{R}^n$ be open Then there is a constant $C > 0$ such that

$$\|u\|_{H_h^2(U)} \le C\left(\|Q(h)u\|_{L^2(W)} + \|u\|_{L^2(W)}\right)$$

for all $u \in \mathscr{S}(\mathbb{R}^n)$.

Proof. Let $u \in \mathscr{S}(\mathbb{R}^n)$ and let $U \subset\subset W \subset \mathbb{R}^n$ be open, and recall that

$$\|u\|^2_{H_h^2(U)} = \|u\|^2_{L^2(U)} + h^2\sum_{j=1}^n\|\partial_j u\|^2_{L^2(U)} + h^4\sum_{k,l=1}^n\|\partial_k\partial_l u\|^2_{L^2(U)}.$$

We will first estimate the term involving $h^2\|\partial_j u\|^2_{L^2(U)}$. Let $\chi \in C_c^\infty(W)$ such that $0 \leq \chi \leq 1$ and $\chi \equiv 1$ on U. (This will allow integration by parts later.) Note that

$$\left(\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)}\right)^2 \leq \left|\langle \chi u, \chi Q(h)u\rangle_{L^2(W)}\right|^2 \leq \|\chi u\|^2_{L^2(W)}\|\chi Q(h)u\|^2_{L^2(W)},$$

by the Cauchy-Schwarz inequality. Hence

$$\begin{aligned}\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)} &\leq \frac{1}{2}\left(\|\chi u\|^2_{L^2(W)} + \|\chi Q(h)u\|^2_{L^2(W)}\right)\\ &\leq \frac{1}{2}\left(\|u\|^2_{L^2(W)} + \|Q(h)u\|^2_{L^2(W)}\right)\end{aligned}$$

where

$$\begin{aligned}&\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)}\\ &\quad = \Re\left(\int_W dx\left[\chi^2(x)\overline{u(x)}\left(-h^2\Delta u(x) + \langle a(x), hDu(x)\rangle + b(x)u(x)\right)\right]\right)\\ &\quad = \int_W dx\left[\langle hD(\chi^2 u)(x), hDu(x)\rangle + \chi^2(x)\Re\left(\overline{u(x)}\langle a(x), hDu(x)\rangle\right) + \chi^2(x)|u(x)|^2\Re(b(x))\right].\end{aligned}$$

Using the fact that χ is compactly supported, we can estimate each of the three terms of $\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)}$ from below:

- $$\begin{aligned}\int_W dx\left[\langle hD(\chi^2 u)(x), hDu(x)\rangle\right] &= \int_W dx\left[\chi^2(x)|hDu(x)|^2 + 2\chi(x)\overline{u(x)}\langle hD\chi(x), hDu(x)\rangle\right]\\ &\geq \int_W dx\left[\chi^2(x)|hDu(x)|^2\right] - C\int_W dx\left[\chi(x)|u(x)||hDu(x)|\right]\\ &\geq \frac{2}{3}\int_W dx\left[\chi^2(x)|hDu(x)|^2\right] - C\int_W dx\left[|u(x)|^2\right],\end{aligned}$$
- $$\begin{aligned}\int_W dx\left[\chi^2(x)\Re\left(\overline{u(x)}\langle a(x), hDu(x)\rangle\right)\right] &\geq -C\int_W dx\left[\chi^2(x)|u(x)||hDu(x)|\right]\\ &\geq -\frac{1}{3}\int_W dx\left[\chi^2(x)|hDu(x)|^2\right] - C\int_W dx\left[|u(x)|^2\right],\end{aligned}$$
- $$\int_W dx\left[\chi^2(x)|u(x)|^2\Re(b(x))\right] \geq -C\int_W dx\left[|u(x)|^2\right].$$

Hence $\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)} \geq \frac{1}{3}\int_W dx\left[\chi^2(x)|hDu(x)|^2\right] - C\int_W dx\left[|u(x)|^2\right]$. Finally, we obtain:

$$\begin{aligned}h^2\sum_{j=1}^n \|\partial_j u\|^2_{L^2(U)} &= \int_U dx\left[|hDu(x)^2|\right] = \int_U dx\left[\chi^2(x)|hDu(x)|^2\right]\\ &\leq \int_W dx\left[\chi^2(x)|hDu(x)|^2\right]\\ &\leq C\Re\langle \chi u, \chi Q(h)u\rangle_{L^2(W)} + C\int_W dx\left[|u(x)|^2\right]\\ &\leq C\|u\|^2_{L^2(W)} + C\|Q(h)u\|^2_{L^2(W)}.\end{aligned}$$

Next, we will estimate the terms involving $h^4\|\partial_k\partial_l u\|^2_{L^2(U)}$. Again, let $\chi \in C_c^\infty(W)$ such that $0 \leq \chi \leq 1$ and $\chi \equiv 1$ on U. Note that

$$\begin{aligned}\sum_{k,l=1}^n \|\partial_k\partial_l(\chi u)\|^2_{L^2(W)} &= \sum_{k,l=1}^n \int_W dx\left[\partial_k\partial_l(\chi\overline{u})(x)\partial_k\partial_l(\chi u)(x)\right] = \sum_{k,l=1}^n \int_W dx\left[\partial_k^2(\chi\overline{u})(x)\partial_l^2(\chi u)(x)\right]\\ &= \int_W dx\left[\Delta(\chi\overline{u})(x)\Delta(\chi u)(x)\right] = \|\Delta(\chi u)\|^2_{L^2(W)}.\end{aligned}$$

Then we have $\Re\langle \chi h^2\Delta u, \chi Q(h)u\rangle_{L^2(W)} \leq \frac{1}{2}(\|h^2\Delta u\|^2_{L^2(W)} + \|Q(h)u\|^2_{L^2(W)})$ and the rest follows as before. $\square$

Theorem 5.8. *(Agmon-Lithner estimate) Let $\lambda \in \mathbb{R}$ and let $U \subset \mathbb{R}^n$ open such that*

$$U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > \lambda\}.$$

Then for all open $W \in \mathbb{R}^n$ such that $U \subset\subset W$, there are constants $h_0, \delta, C > 0$ such that

$$\|u\|_{L^2(U)} \leq Ce^{-\delta/h}\|u\|_{L^2(W)} + C\|(P(h) - \lambda)u\|_{L^2(W)}$$

for all $u \in H^1(\mathbb{R}^n)$ and all $0 < h \leq h_0$.

Proof. We can assume without loss of generality that $W \subset\subset \{x \in \mathbb{R}^n \mid V(x) > \lambda\}$. We can choose functions $\varphi, \psi, \chi \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq \varphi, \psi, \chi \leq 1$ and

$$\begin{aligned} &\psi \equiv 1 \text{ on } U, \\ &\varphi \equiv 1 \text{ on } \mathrm{Supp}(\psi), \\ &\chi \equiv 1 \text{ on } \mathrm{Supp}(\varphi), \text{ and} \\ &\mathrm{Supp}(\chi) \subset\subset W. \end{aligned}$$

Observe that $V(x) - \lambda > 0$ and $|\partial\psi(x)| < C$ for all $x \in W$ and some $C > 0$. Then we can pick $\delta > 0$ small enough such that $V(x) - \lambda - \delta^2|\partial\psi(x)|^2 > 0$ for all $x \in W$. Hence for all $x \in W$,

$$|p_{\delta\psi}(x,\xi) - \lambda|^2 = \left||\xi|^2 + 2\delta i\langle\partial\psi(x), \xi\rangle + V(x) - \lambda - \delta^2|\partial\psi(x)|^2\right|^2 \geq V(x) - \lambda - \delta^2|\partial\psi(x)|^2 > 0.$$

Choose $\sigma > 0$ such that $|p_{\delta\psi}(x,\xi) - \lambda|^2 \geq \sigma^2$ and let $m_{k,l}(x,\xi) := \langle x\rangle^k\langle\xi\rangle^l$. Since χ is compactly supported, we have $(p_{\delta\psi} - \lambda)\#\chi \in S(m_{0,2})$, and so $((p_{\delta\psi} - \lambda)\#\chi)\#m_{0,-2} \in S$. Then we can define

$$\begin{aligned} b &:= \overline{((p_{\delta\psi} - \lambda)\#\chi)\#m_{0,-2}}\#\left[((p_{\delta\psi} - \lambda)\#\chi)\#m_{0,-2}\right] - \sigma^2\overline{\chi\#m_{0,-2}}\#[\chi\#m_{0,-2}] \\ &= \left[m_{0,-2}\#(\chi\#\overline{p_{\delta\psi} - \lambda})\right]\#\left[((p_{\delta\psi} - \lambda)\#\chi)\#m_{0,-2}\right] - \sigma^2[m_{0,-2}\#\chi]\#[\chi\#m_{0,-2}]. \end{aligned}$$

Then $b \in S$, b is real-valued by remark 4.32, and

$$b(x,\xi) = \langle\xi\rangle^{-4}\chi(x)^2|p_{\delta\psi} - \lambda|^2 - \sigma^2\langle\xi\rangle^{-4}\chi(x)^2 + O_S(h) \geq -h\gamma$$

for some constant $\gamma > 0$. Hence by the Gårding inequality, we obtain $\langle u, b^W(x,hD)u\rangle_{L^2(\mathbb{R}^n)} \geq -h\gamma\|u\|^2_{L^2(\mathbb{R}^n)}$ for all $u \in L^2(\mathbb{R}^n)$. Let $u := (1 + h^2\Delta)(\varphi v)$ for some $v \in \mathscr{S}(\mathbb{R}^n)$, then $m_{0,-2}(x,hD)u(x) = \varphi(x)v(x)$ (as can be shown with an easy computation), and so

$$\begin{aligned} -h\gamma\|(1 + h^2\Delta)(\varphi v)\|^2_{L^2(\mathbb{R}^n)} &\leq \langle(p^W_{\delta\phi}(x,hD) - \lambda)(\chi\varphi v), (p^W_{\delta\phi}(x,hD) - \lambda)(\chi\varphi v)\rangle - \sigma^2\langle\chi\varphi v, \chi\varphi v\rangle \\ &= \|(p^W_{\delta\psi}(x,hD) - \lambda)(\varphi v)\|^2_{L^2(\mathbb{R}^n)} - \sigma^2\|\varphi v\|^2_{L^2(\mathbb{R}^n)}, \end{aligned}$$

where we used that $\overline{a}^W(x,hD) = a^W(x,hD)^*$ and $\chi \equiv 1$ on $\mathrm{Supp}(\varphi)$. Now by proposition 5.7 we can estimate

$$\begin{aligned} \|(1 + h^2\Delta)(\varphi v)\|_{L^2(\mathbb{R}^n)} &\leq C\|\varphi v\|_{H^2_h(\mathbb{R}^n)} = C\|\varphi v\|_{H^2_h(\mathrm{Supp}(\varphi))} \\ &\leq C\left(\|\varphi v\|_{(W)} + \|(p^W_{\delta\varphi}(x,hD) - \lambda)(\varphi v)\|_{L^2(W)}\right) \\ &= C\left(\|\varphi v\|_{L^2(\mathbb{R}^n)} + \|(p^W_{\delta\varphi}(x,hD) - \lambda)(\varphi v)\|_{L^2(\mathbb{R}^n)}\right), \end{aligned}$$

and so

$$\|(1 + h^2\Delta)(\varphi v)\|^2_{L^2(\mathbb{R}^n)} \leq C\left(\|\varphi v\|^2_{L^2(\mathbb{R}^n)} + \|(p^W_{\delta\varphi}(x,hD) - \lambda)(\varphi v)\|^2_{L^2(\mathbb{R}^n)}\right).$$

Combining this with the previous estimate we obtain

$$\|(p^W_{\delta\psi}(x,hD) - \lambda)(\varphi v)\|^2_{L^2(\mathbb{R}^n)} \geq \frac{\sigma^2 - hC}{1 + hC}\|\varphi v\|^2_{L^2(\mathbb{R}^n)} \geq \frac{\sigma^2}{4}\|\varphi v\|^2_{L^2(\mathbb{R}^n)}$$

for all $0 < h \leq h_0$ for some sufficiently small $h_0 > 0$. Let $w \in \mathscr{S}(\mathbb{R}^n)$, then $v := e^{\delta\psi/h}w \in \mathscr{S}(\mathbb{R}^n)$ since ψ is compactly supported. Then the previous estimate becomes

$$\begin{aligned} \|e^{\delta\psi/h}\varphi w\|_{L^2(\mathbb{R}^n)} &\leq C\|(p^W_{\delta\psi}(x,hD) - \lambda)(e^{\delta\psi/h}\varphi w)\|_{L^2(\mathbb{R}^n)} = C\|e^{\delta\psi/h}(p^W(x,hD) - \lambda)(\varphi w)\|_{L^2(\mathbb{R}^n)} \\ &\leq C\left(\|e^{\delta\psi/h}\varphi(p^W(x,hD) - \lambda)w\|_{L^2(\mathbb{R}^n)} + \|e^{\delta\psi/h}[p^W(x,hD), \varphi]w\|_{L^2(\mathbb{R}^n)}\right), \end{aligned}$$

where

$$[p^W(x,hD),\varphi]w := p^W(x,hD)(\varphi w) - \varphi p^W(x,hD)w$$

is the commutator. Due to $\varphi \equiv 1$ on $\mathrm{Supp}(\psi)$, we have $\psi \equiv 0$ on $\mathrm{Supp}([p^W(x,hD),\varphi]w)$. Then

$$\begin{aligned}
\|e^{\delta\psi/h}[p^W(x,hD),\varphi]w\|_{L^2(\mathbb{R}^n)} &= \|[p^W(x,hD),\varphi]w\|_{L^2(\mathbb{R}^n)} \\
&= \|-h^2\Delta(\varphi w) + \varphi h^2 \Delta w\|_{L^2(\mathbb{R}^n)} \\
&= \||hD|^2(\varphi)w + 2\langle hD\varphi, hDw\rangle\|_{L^2(\mathbb{R}^n)} \\
&\leq \|w\|_{H_h^2(\mathrm{Supp}(\varphi))} \\
&\leq C\|w\|_{L^2(W)} + C\|(p^W(x,hD)-\lambda)w\|_{L^2(W)}.
\end{aligned}$$

Hence for all $w \in \mathscr{S}(\mathbb{R}^n)$, using that $\varphi \equiv \psi \equiv 1$ on U,

$$\begin{aligned}
\|w\|_{L^2(U)} &= e^{-\delta/h}\|e^{\delta/h}w\|_{L^2(U)} = e^{-\delta/h}\|e^{\delta\psi/h}\varphi w\|_{L^2(U)} \\
&\leq e^{-\delta/h}\|e^{\delta\psi/h}\varphi w\|_{L^2(\mathbb{R}^n)} \\
&\leq e^{-\delta/h}C\|w\|_{L^2(W)} + (e^{-\delta/h}+1)C\|(p^W(x,hD)-\lambda)w\|_{L^2(W)} \\
&\leq e^{-\delta/h}C\|w\|_{L^2(W)} + C\|(p^W(x,hD)-\lambda)w\|_{L^2(W)}.
\end{aligned}$$

for all $0 < h \leq h_0$ for some $h_0 > 0$. □

In the proof of the Agmon-Lithner estimate, we assumed that $\delta > 0$ is small enough so that we have $V(x) - \lambda - \delta^2|\partial\psi(x)|^2 > 0$ for all $x \in W \subset\subset \{x \in \mathbb{R}^n \mid V(x) > \lambda\}$ where $\psi \in C_c^\infty(\mathbb{R}^n)$ is some function so that $\psi \equiv 1$ on U and $\mathrm{Supp}(\psi) \subset W$. We can rewrite this condition to

$$\delta|\partial\psi(x)| < \sqrt{V(x)-\lambda}$$

for all $x \in W$.

We will now consider smooth curves $\gamma : [0.1] \to \overline{W}$ such that $\gamma(0) \in U$ and $\gamma(1) \in \partial W$. Integrating both sides along γ gives

$$\delta \int_\gamma dx\,[|\partial\psi(x)|] < \int_\gamma dx\left[\sqrt{V(x)-\lambda}\right].$$

This motivates the following definition.

Definition 5.9. *(Agmon metric) Let $W \subset \mathbb{R}^n$ and let $V : W \to [0,\infty)$ be a smooth function. Then the Agmon-metric d_V is defined by*

$$d_V(x,y) := \inf\left\{\int_\gamma dx\left[\sqrt{V(x)}\right] \mid \gamma \in C^\infty([0,1],W), \gamma(0)=x, \gamma(1)=y\right\} \tag{5.5}$$

for all $x, y \in W$. Furthermore, we define

$$d_V(x,U) := \inf_{y\in Y} d_V(x,y) \tag{5.6}$$

where $x \in W$ and $U \subseteq W$, and

$$\begin{aligned}
d_V(U_1,U_2) &:= \inf_{x\in U_1} d_V(x,U_2) &(5.7)\\
&= \inf\{\int_\gamma dx\left[\sqrt{V}\right] \mid \gamma \in C^\infty([0,1],W), \gamma(0)\in U_1, \gamma(1) \in U_2\} &(5.8)
\end{aligned}$$

for all $U_1, U_2 \subseteq W$.

Lemma 5.10. *Let $U \subset\subset W \subset\subset \{x \in \mathbb{R}^n \mid V(x) > \lambda\}$ and let $\delta > 0$. Then the following two statements are equivalent:*

(i) $\exists\psi \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq \psi \leq 1$, $\psi \equiv 1$ on U, Supp$(\psi) \subseteq W$, and

$$\delta|\partial\psi(x)| < \sqrt{V(x)-\lambda}$$

for all $x \in W$.

(ii) $\delta < d_{V-\lambda}(U, \partial W)$

Proof. ((i) $\implies$ (ii)) We have for all $x \in W$ that $\delta|\partial\psi(x)| < \sqrt{V(x)-\lambda}$. But $\overline{W}$ is compact, so there is some $\epsilon > 0$ such that

$$\delta|\partial\psi(x)| < \sqrt{V(x)-\lambda} - \frac{\epsilon}{d(U,\partial W)}$$

for all $x \in W$, where $d(U,\partial W) > 0$ is the distance between U and ∂W in the Euclidean metric.

Let $\gamma : [0,1] \to \{x \in \mathbb{R}^n \mid V(x) > \lambda\}$ be a smooth curve such that $\gamma(0) \in U, \gamma(1) \in \partial W$. Since $\psi(\gamma(0)) = 1$ and $\psi(\gamma(1)) = 0$, we have $\int_\gamma dx\,[|\partial\psi(x)|] \geq 1$. Hence

$$\delta \leq \delta \int_\gamma [|\partial\psi(x)|] < \int_\gamma dx \left[\sqrt{V(x)-\lambda}\right] - \frac{\epsilon}{d(U,\partial W)} \int_\gamma dx\,[1] < \int_\gamma dx \left[\sqrt{V(x)-\lambda}\right] - \epsilon.$$

So $\delta \leq d_{V-\lambda}(U,\partial W) - \epsilon < d_{V-\lambda}(U,\partial W)$.

((ii) $\implies$ (i)) Let $\delta < d_{V-\lambda}(U,\partial W)$. We need to find a suitable function ψ such that for all $x \in W$, $\delta|\partial\psi(x)| < \sqrt{V(x)-\lambda}$. We would like to take

$$\tilde{\psi}(x) := \max\left(0, 1 - \frac{d_{V-\lambda}(x,U)}{d_{V-\lambda}(U,\partial W)}\right),$$

but this function is certainly not smooth. Since $\delta < d_{V-\lambda}(U,\partial W)$, there are $0 < \tilde{\epsilon} < \epsilon$ such that $(1+\tilde{\epsilon})\delta < d_{V-\lambda}(U,\partial W) - \epsilon$. Then we can define the function $\tilde{\psi}_\epsilon$ by

$$\tilde{\psi}_\epsilon(x) = \max\left(0, 1 - \frac{d_{V-\lambda}(x,U) - \epsilon/2}{d_{V-\lambda}(U,\partial W) - \epsilon}\right).$$

Finally, we can smoothen this by mollification to obtain $\psi \in C_c^\infty(\mathbb{R}^n)$ such that $\psi(x) \equiv 1$ on U, $\mathrm{Supp}(\psi) \subseteq W$, $0 \leq \psi \leq 1$, and

$$|\partial\psi(x)| < \frac{(1+\tilde{\epsilon})}{d_{V-\lambda}(U,\partial W) - \epsilon}\sqrt{V(x)-\lambda}$$

for all $x \in W$. Then

$$\delta|\partial\psi(x)| < \frac{\delta(1+\tilde{\epsilon})}{d_{V-\lambda}(U,\partial W) - \epsilon}\sqrt{V(x)-\lambda} < \sqrt{V(x)-\lambda}$$

as desired. □

Theorem 5.11. *(Exponential decay) Let $u \in H^1(\mathbb{R}^n)$ such that $P(h)u = E(h)u$. Let $E = \lim_{h\to 0} E(h)$ and $U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > E\}$. Let*

$$\delta_0 := d_{V-E}(U, \{x \in \mathbb{R}^n \mid V(x) = E\}).$$

Then for all $\delta < \delta_0$ we have

$$\|u\|_{L^2(U)} \leq e^{-\delta/h} \tag{5.9}$$

as $h \to 0$.

Proof. Let $\delta < \delta' < \delta_0$. Since $\overline{U}$ is compact, we have $\inf_{x\in U} V(x) - E > 0$. Then

$$U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > E(h)\}$$

if $h > 0$ is sufficiently small. By the Agmon-Lithner estimate, we have $\|u\|_{L^2(\mathbb{R}^n)} \leq Ce^{-\delta'/h} \leq e^{-\delta/h}$ as $h \to 0$. □

5.3 Carleman inequality

We will now estimate $\|u\|_{L^2(U)}$ from below, where u is again a solution to the Schrödinger equation and $U \subset\subset \{x \in \mathbb{R}^n \mid V(x) > E\}$ for some energy level E. Our goal is to show that $\|u\|_{L^2(U)} \geq e^{-\gamma/h}$ for some sufficiently large $\gamma > 0$.

As we have seen in the proof of the Agmon-Lithner estimate, it makes sense to consider symbols of the form $\overline{a}\#a$, because they satisfy $\langle u, (\overline{a}\#a)^W(x, hD)u\rangle = \|a^W(x, hD)u\|^2$. We will now combine this with the first-order approximation from corollary 4.31, i.e.

$$\begin{aligned}\overline{a}\#a &= |a|^2 + \frac{h}{2i}\{\overline{a}, a\} + O_{S(m^2)}(h^2) = |a|^2 + \frac{1}{2}hi\{a, \overline{a}\} + O_{S(m^2)}(h^2)\\ &\geq \frac{h}{2}\left(\frac{2}{h_0}|a|^2 + i\{a, \overline{a}\}\right) + O_{S(m^2)}(h^2).\end{aligned}$$

We want to set $a = p_\varphi$ and apply the Gårding inequality to the symbol $\frac{2}{h_0}|p_\varphi|^2 + i\{p_\varphi, \overline{p_\varphi}\}$. (Note that this symbol is real-valued.) Since we already know that $\langle u, (\overline{p_\varphi}\#p_\varphi)^W(x, hD)u\rangle = \|p_\varphi^W(x, hD)u\|^2 \geq 0$, this approach only yields a stronger result if

$$\inf\left(\frac{2}{h_0}|p_\varphi|^2 + i\{p_\varphi, \overline{p_\varphi}\}\right) > 0.$$

As before, we will have to work around the fact that p_φ is unbounded. Let $W \subset\subset \mathbb{R}^n$ and let $\tilde{\chi}, \chi \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq, \tilde{\chi}, \chi \leq 1$ and $\tilde{\chi} \equiv 1$ on W, $\chi \equiv 1$ on $\mathrm{Supp}(\tilde{\chi})$, and define $q_\varphi := p_\varphi\#\chi\#m_{0,-2}$. Then $q_\varphi \in S$, and

$$|q_\varphi(x, \xi)|^2 = |p_\varphi(x, \xi)|^2\chi(x)^2\langle\xi\rangle^{-4} + O_S(h).$$

Combining the previous equations, we obtain

$$\begin{aligned}\overline{q_\varphi}\#q_\varphi &\geq \frac{h}{2}\left(\frac{2}{h_0}|q_\varphi|^2 + i\{q_\varphi, \overline{q_\varphi}\}\right) + O_S(h^2)\\ &= \frac{h}{2}\left(\frac{2}{h_0}|p_\varphi|^2\chi^2 m_{0,-2}^2 + i\{q_\varphi, \overline{q_\varphi}\}\right) + O_S(h^2).\end{aligned} \tag{5.10}$$

We will now consider the symbol $\frac{2}{h_0}|p_\varphi|^2\chi^2 m_{0,-2}^2 + i\{q_\varphi, \overline{q_\varphi}\} \in S$, and prove that there is a constant $\sigma > 0$ such that

$$\frac{2}{h_0}|p_\varphi|^2\chi^2 m_{0,-2}^2 - \sigma^2\chi^2 m_{0,-2}^2 + i\{q_\varphi, \overline{q_\varphi}\} \geq 0$$

under the additional assumption that $i\{p_\varphi, \overline{p_\varphi}\}(x, \xi) > 0$ whenever $p_\varphi(x, \xi) = 0$.

(i) Since $|p_\varphi|$ is quadratic in $|\xi|$, there is for each $x \in \mathbb{R}^{2n}$ a sufficiently small constant $\sigma_x > 0$ such that $|p_\varphi(x, \xi)|^2\langle\xi\rangle^{-4} > \sigma_x^2$ if $|\xi|$ is sufficiently large. But $\mathrm{Supp}(\chi)$ is compact, so there are a sufficiently small $\sigma > 0$ and a sufficiently large R such that $|p(x, \xi)|^2\langle\xi\rangle^{-4} > \sigma^2$ for all $(x, \xi) \in \mathrm{Supp}(\chi) \times \mathbb{R}^n \backslash B(0, R)$.

Then $|p_\varphi(x, \xi)|^2\chi(x)^2\langle\xi\rangle^{-4} - \sigma^2\chi(x)^2\langle\xi\rangle^{-4} \geq 0$ for all $x \in \mathbb{R}^n$, and so there is a sufficiently small constant $h_0 > 0$ such that

$$\frac{2}{h_0}|p_\varphi(x, \xi)|^2\chi(x)^2\langle\xi\rangle^{-4} - \sigma^2\chi(x)^2\langle\xi\rangle^{-4} + i\{q_\varphi, \overline{q_\varphi}\}(x, \xi) \geq 0$$

for all $(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n \backslash B(0, R)$, where we used that $i\{q_\varphi, \overline{q_\varphi}\}$ is bounded and supported on $\mathrm{Supp}(\chi) \times \mathbb{R}^n$.

(ii) If $\xi \in B(0, R)$, it may happen that $|p_\varphi(x, \xi)| = 0$. In the case, we need $i\{q_\varphi, \overline{q_\varphi}\} > 0$. We have

$$\begin{aligned}\{q_\varphi, \overline{q_\varphi}\} &= |\chi\#m_{0,-2}|^2\{p_\varphi, \overline{p_\varphi}\} + (\chi\#m_{0,-2})\overline{p_\varphi}\{p_\varphi, \overline{\chi\#m_{0,-2}}\}\\ &+ \overline{\chi\#m_{0,-2}}p_\varphi\{\chi\#m_{0,-2}, \overline{p_\varphi}\} + |p_\varphi|^2\{\chi\#m_{0,-2}, \overline{\chi\#m_{0,-2}}\} + O_S(h).\end{aligned}$$

So if assume that $p(x,\xi) = 0 \Longrightarrow i\{p_\varphi, \overline{p_\varphi}\} > 0$ for all $(x,\xi) \in \overline{W} \times \mathbb{R}^n$, then we have $i\{q_\varphi, \overline{q_\varphi}\} > 0$ for all $0 < h \le h_0$ where $h_0 > 0$ is sufficiently small. Define $N := \{(x,\xi) \in W \times \mathbb{R}^n \mid |p_\varphi(x,\xi)| = 0\}$. Note that $N \subset \operatorname{Supp}(\chi) \times B(0,R) \subset\subset \mathbb{R}^{2n}$. Let $\epsilon > 0$ and define

$$N_\epsilon := \bigcup_{z \in N} B(z, \epsilon).$$

Since $\{q_\varphi, \overline{q_\varphi}\}$ is continuous and $\overline{N}$ is compact, there is $\epsilon_0 > 0$ such that $i\{q_\varphi, \overline{q_\varphi}\} > 0$ on $\overline{N_{\epsilon_0}}$. Then there is a $\sigma > 0$ such that for all $(x,\xi) \in N_{\epsilon_0}$,

$$\frac{2}{h_0}|p_\varphi(x,\xi)|^2 \chi(x)^2 \langle\xi\rangle^{-4} + i\{q_\varphi, \overline{q_\varphi}\}(x,\xi) - \sigma^2 \chi(x)^2 \langle\xi\rangle^{-4} \ge i\{q_\varphi, \overline{q_\varphi}\}(x,\xi) - \sigma^2 \chi(x)^2 \langle\xi\rangle^{-4} \ge 0.$$

(iii) Finally, $\overline{\operatorname{Supp}(\chi) \times B(0,R)} \backslash N_{\epsilon_0}$ is compact and $|p_\varphi| > 0$ on this domain. So again, there is a constant $\sigma > 0$ such that for all $(x,\xi) \in (\mathbb{R}^n \times B(0,R)) \backslash N_{\epsilon_0}$,

$$\frac{2}{h_0}|p_\varphi(x,\xi)|^2 \chi(x)^2 \langle\xi\rangle^{-4} - \sigma^2 \chi(x)^2 \langle\xi\rangle^{-4} + i\{q_\varphi, \overline{q_\varphi}\}(x,\xi) \ge 0$$

where $h_0 > 0$ is sufficiently small.

Hence

$$\frac{2}{h_0}|p_\varphi(x,\xi)|^2 \chi(x)^2 \langle\xi\rangle^{-4} + i\{q_\varphi, \overline{q_\varphi}\}(x,\xi) - \sigma^2 \chi(x)^2 \langle\xi\rangle^{-4} \ge 0 \tag{5.11}$$

on all of $\mathbb{R}^{2n}$. So if $h_0 > 0$ is sufficiently small, then for all $0 < h \le h_0$ we have

$$\frac{2}{h_0}|p_\varphi(x,\xi)|^2 \chi(x)^2 \langle\xi\rangle^{-4} + i\{q_\varphi, \overline{q_\varphi}\}(x,\xi) - \sigma^2 \overline{\chi \# m_{0,-2}} \# \chi \# m_{0,-2} \ge 0. \tag{5.12}$$

We will now repeat the last steps of the proof of the Agmon-Lithner estimate. We apply the Gårding-inequality, set $u := (1 + h^2\Delta)(\tilde{\chi} v)$ for $v \in \mathscr{S}$, and apply proposition 5.7. Then

$$\begin{aligned}
\langle u, \left(\frac{2}{h_0}|q_\varphi|^2 + i\{q_\varphi, \overline{q_\varphi}\}\right)^W (x,hD)u\rangle &\ge \sigma^2 \|\chi m_{0,-2}^W(x,hD)u\|^2 - h\gamma\|u\|^2, \\
\|q_\varphi^W(x,hD)u\|^2 &= \langle u, (\overline{q_\varphi} \# q_\varphi)^W (x,hD)u\rangle \\
&= \langle u, (|q_\varphi|^2)^W (x,hD)u\rangle + h\langle u, \frac{1}{2} i\{q_\varphi, \overline{q_\varphi}\}^W (x,hD)u\rangle + O(h^2)\|u\| \\
&\ge \frac{h}{2}\langle u, \left(\frac{2}{h_0}|q_\varphi|^2 + i\{q_\varphi, \overline{q_\varphi}\}\right)^W (x,hD)u\rangle - h^2 C\|u\|^2 \\
&\ge h\frac{\sigma^2}{2}\|\chi m_{0,-2}^W(x,hD)u\|^2 - h^2 C\|u\|^2, \\
\|p_\varphi^W(x,hD)(\tilde{\chi} v)\|^2 &= \|p_\varphi^W(x,hD)(\chi\tilde{\chi} v)\|^2 \\
&\ge h\frac{\sigma^2}{2}\|\chi\tilde{\chi} v\|^2 - h^2 C\|(1 + h^2\Delta)(\tilde{\chi} v)\|^2 \\
&\ge h\frac{\sigma^2}{2}\|\tilde{\chi} v\|^2 - h^2 C\left(\|\tilde{\chi} v\|^2 + \|p_\varphi^W(x,hD)(\tilde{\chi} v)\|^2\right) \\
&\ge h\frac{\sigma^2}{4}\|\tilde{\chi} v\|^2
\end{aligned}$$

for all $0 < h \le h_0$ if $h_0 > 0$ is sufficiently small. Then

$$\sqrt{h}\|v\|_{L^2(W)} \le C\|p_\varphi^W(x,hD)(\tilde{\chi} v)\|_{L^2(\mathbb{R}^n)}.$$

Since this holds for any $\tilde{\chi}$ such that $\overline{W} \subset \operatorname{Supp}(\tilde{\chi})$, we obtain

$$\sqrt{h}\|v\|_{L^2(W)} \le C\|p_\varphi^W(x,hD)v\|_{L^2(W)}.$$

This motivates the following definition and proves the following proposition.

Definition 5.12. *(Hörmander's hypoellipticity condition) Let $\varphi : \mathbb{R}^n \to \mathbb{C}$ be smooth and let $W \subset \mathbb{R}^n$. Then p_φ is said to satisfy Hörmander's hypoellipticity condition within W if*

$$p_\varphi(x, \xi) = 0 \Longrightarrow i\{p_\varphi, \overline{p_\varphi}\}(x, \xi) > 0 \tag{5.13}$$

for all $(x, \xi) \in W \times \mathbb{R}^n$.

Proposition 5.13. *Let $W \subset\subset \mathbb{R}^n$ and assume that p_φ satisfies Hörmander's hypoellipticitiy condition within $\overline{W}$. Then there exists a sufficiently large constant $C > 0$ and a sufficiently small constants $h_0 > 0$ such that*

$$h^{1/2}\|u\|_{L^2(W)} \leq C\|p_\varphi^W(x, hD)u\|_{L^2(W)}$$

for all $u \in \mathscr{S}(\mathbb{R}^n)$ and all $0 < h \leq h_0$.

As it turns out, for any $W \subset\subset \mathbb{R}^n$, we can pick a suitable function φ such that p_φ satisfies Hörmander's hypoellipticity condition within W.

Proposition 5.14. *For all $0 < r < R$ there is a positive, nonincreasing, radial function $\varphi \in C^\infty(\mathbb{R}^n)$ such that p_φ satisfies Hörmander's hypoellipticity condition within $B(0, R)\backslash B(0, r)$.*

Theorem 5.15. *(Carleman estimate) Let $a < b$ and let $U \subset\subset \mathbb{R}^n$. Let $V \in S(m_{k,0})$. Let u be a solution of the Schrödinger equation such that $a < E(h) < b$ for all $0 < h \leq h_0$ for some $h_0 > 0$. Assume further that $p - b \in S(m_{k,2})$ is elliptic for $|x| \geq R$ for some sufficiently large $R > 0$. Then there is a constant $\gamma > 0$ such that for all $0 < h \leq h_0$;*

$$\|u\|_{L^2(U)} \geq e^{-\gamma/h}. \tag{5.14}$$

Remark 5.16. *The ellipticity condition means that there is are constants $\gamma, R > 0$ such that $V(x) \geq \gamma\langle x\rangle^k$ for all $|x| \geq R$ in case $k > 0$, or $V(x) - b \geq \gamma$ for all $|x| \geq R$ in case $k = 0$.*

Proof. Without loss of generality we may assume that $0 \in U$. (If not, we can pick $x_0 \in U$ and shift the entire problem, i.e. set $\tilde{x} := x - x_0$.) Then there is a sufficiently small $r > 0$ such that $B(0, 3r) \subset U$. It sufficies to prove the theorem for $U = B(0, 3r)$. We may also assume without loss of generality that R is large enough such that $3r < R - 5$.

Let $V_0 \in C_c^\infty(\mathbb{R}^n)$ be some dummy potential such that $\text{Supp}(V_0) \subset B(0, R)$ and $p(x, \xi) - b + V_0(x) \neq 0$ for all $(x, \xi) \in \mathbb{R}^{2n}$. Then $p - b + V_0$ is elliptic on all of $\mathbb{R}^{2n}$, and hence also $p - E + V_0$. By proposition 5.2 there are $h_0, C > 0$ such that for all $v \in L^2(\mathbb{R}^n)$, for all $0 < h \leq h_0$;

$$\|v\|_{L^2(\mathbb{R}^n)} \leq C\|(p^W(x, hD) + V_0 - E)v\|_{L^2(\mathbb{R}^n)}.$$

If we assume that $\text{Supp}(v) \subset \mathbb{R}^n\backslash B(0, R)$, this reduces to

$$\|v\|_{L^2(\mathbb{R}^n)} \leq C\|(p^W(x, hD) - E)v\|_{L^2(\mathbb{R}^n)}. \tag{5.15}$$

Now define $\chi_1, \chi_2 \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq \chi_1, \chi_2 \leq 1$ and

$$\begin{aligned}
&\chi_1 \equiv 0 \text{ on } B(0, r) \cup \mathbb{R}^n\backslash B(0, R),\\
&\chi_1 \equiv 1 \text{ on } B(0, R - 1)\backslash B(0, 2r),\\
&\chi_2 \equiv 0 \text{ on } B(0, R - 4),\\
&\chi_2 \equiv 1 \text{ on } \mathbb{R}^n\backslash B(0, R - 3).
\end{aligned}$$

The functions χ_1 and χ_2 were picked so that for all $x_0 \in \mathbb{R}^n\backslash U$, we have $\chi_j \equiv 1$ on $B(x_0, 1/2)$ for at least one of the two. Hence $\|u\|_{L^2(\mathbb{R}^n)} \leq \|u\|_{L^2(U)} + \|u\|_{L^2(\mathbb{R}^n\backslash U)} \leq \|u\|_{L^2(U)} + \|\chi_1 u\|_{L^2(\mathbb{R}^n)} + \|\chi_2 u\|_{L^2(\mathbb{R}^n)}$. Our goal is to estimate the sum $\|\chi_1 u\|_{L^2(\mathbb{R}^n)} + \|\chi_2 u\|_{L^2(\mathbb{R}^n)}$ from above in terms of $\|u\|_{L^2(U)}$.

Note that for any $\chi \in C_c^\infty(\mathbb{R}^n)$, we have

$$\begin{aligned}
(p^W(x, hD) - E)(\chi u) &= \chi(p^W(x, hD) - E)u + [p^W(x, hD) - E, \chi]u\\
&= [p^W(x, hD), \chi]u\\
&= -h^2\Delta(\chi u) + h^2\chi\Delta u\\
&= -h^2 u\Delta\chi - 2h^2\langle\partial\chi, \partial u\rangle,
\end{aligned}$$

and so

$$\|(p^W(x,hD)-E)(\chi u)\|_{L^2(\mathbb{R}^n)} \le Ch\|u\|_{H^1_h(\mathrm{Supp}(\chi))}. \tag{5.16}$$

Then we can apply (5.15) to $v := \chi_2 u$ to obtain

$$\begin{aligned}
\|\chi_2 u\|_{L^2(\mathbb{R}^n)} &\le C\|(p^W(x,hD)-E)(\chi_2 u)\|_{L^2(\mathbb{R}^n)}\\
&\le Ch\|u\|_{H^1_h(B(0,R-3)\backslash B(0,R-4))}\\
&\le Ch\|u\|_{H^2_h(B(0,R-3)\backslash B(0,R-4))}\\
&\le Ch\left(\|(p^W(x,hD)-E)u\|_{L^2(B(0,R-2)\backslash B(0,R-5))}+\|u\|_{L^2(B(0,R-2)\backslash B(0,R-5))}\right)\\
&= Ch\|u\|_{L^2(B(0,R-2)\backslash B(0,R-5))}\\
&= Ch\|\chi_1 u\|_{L^2(B(0,R-2)\backslash B(0,R-5))}\\
&\le Ch\|\chi_1 u\|_{L^2(\mathbb{R}^n)}
\end{aligned}$$

where we used proposition 5.7 and the fact that $(p^W(x,hD)-E)u=0$.

By proposition 5.14, there is a positive, nonincreasing radial function $\varphi \in C^\infty(\mathbb{R}^n)$ such that $p_\varphi - E$ satisfies Hörmander's hypoellipticity condition within $W := B(0,R)\backslash B(0,r)$. Then, by proposition 5.13, we have

$$\begin{aligned}
h^{1/2}\|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} &= h^{1/2}\|e^{\varphi/h}\chi_1 u\|_{L^2(W)}\\
&\le C\|(p^W_\varphi(x,hD)-E)(e^{\varphi/h}\chi_1 u)\|_{L^2(W)}\\
&= C\|e^{\varphi/h}(p^W(x,hD)-E)(\chi_1 u)\|_{L^2(W)}\\
&\le Ch\|e^{\varphi/h}u\|_{H^1_h(\mathrm{Supp}(\chi_1))}\\
&= Ch\left(\|e^{\varphi/h}u\|_{H^1_h(B(0,2r)\backslash B(0,r))}+\|e^{\varphi/h}u\|_{H^1_h(B(0,R)\backslash B(0,R-1))}\right)\\
&\le Ch\left(e^{\varphi(r)/h}\|u\|_{H^1_h(B(0,2r)\backslash B(0,r))}+e^{\varphi(R-1)/h}\|u\|_{H^1_h(B(0,R)\backslash B(0,R-1))}\right)\\
&\le Ch\left(e^{\varphi(r)/h}\|u\|_{H^2_h(B(0,2r)\backslash B(0,r))}+e^{\varphi(R-1)/h}\|u\|_{H^2_h(B(0,R)\backslash B(0,R-1))}\right)\\
&\le Ch\left(e^{\varphi(r)/h}\|u\|_{L^2(U)}+e^{\varphi(R-1)/h}\|u\|_{L^2(B(0,R+1)\backslash B(0,R-2))}\right)\\
&\le Ch\left(e^{\varphi(r)/h}\|u\|_{L^2(U)}+e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}\right),
\end{aligned}$$

so we obtain

$$\|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} \le Ch^{1/2}\left(e^{\varphi(r)/h}\|u\|_{L^2(U)}+e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}\right) \tag{5.17}$$

But φ is non-increasing, so $e^{\varphi(R-1)/h}\|\chi_1 u\|_{L^2(\mathbb{R}^n)} \le \|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} + e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}$. So

$$e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)} \le Che^{\varphi(R-1)/h}\|\chi_1 u\|_{L^2(\mathbb{R}^n)} \le Ch\|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} + Che^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}.$$

Combining everything, we finally get

$$\begin{aligned}
&\|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} + e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}\\
&\le Ch^{1/2}e^{\varphi(r)/h}\|u\|_{L^2(U)} + Ch^{1/2}e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)} + Ch\|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} + Che^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}\\
&\le Ch^{1/2}e^{\varphi(r)/h}\|u\|_{L^2(U)}
\end{aligned}$$

for all $0 < h \le h_0$ if $h_0 > 0$ is sufficiently small. Hence

$$\begin{aligned}
\|u\|_{L^2(\mathbb{R}^n)} &\le \|u\|_{L^2(U)} + \|\chi_1 u\|_{L^2(\mathbb{R}^n)} + \|\chi_2 u\|_{L^2(\mathbb{R}^n)}\\
&\le \|u\|_{L^2(U)} + \|e^{\varphi/h}\chi_1 u\|_{L^2(\mathbb{R}^n)} + e^{\varphi(R-1)/h}\|\chi_2 u\|_{L^2(\mathbb{R}^n)}\\
&\le \left(1+Ce^{\varphi(r)/h}\right)\|u\|_{L^2(U)},
\end{aligned}$$

and therefore there are constants $h_0 > 0, \gamma > 0$ such that for all $0 < h \le h_0$, we have

$$\|u\|_{L^2(U)} \ge e^{-\gamma/h}\|u\|_{L^2(\mathbb{R}^n)} = e^{-\gamma/h}. \tag{5.18}$$

□

6 Multiple potential wells

In this section we shall consider the Schrödinger operator $P(h) := -h^2\partial_x^2 + V(x)$ for the potential

$$V(x) := (x^2 - 1)^2.$$

For eigenvalues $E(h) < 1$, the classically permitted domain $\{x \in \mathbb{R} \mid V(x) < E(h)\}$ is split into two connected components, the so-called potential wells.

By the Agmon-Lithner inequality, the eigenfunctions associated with such eigenvalues are exponentially small outside these wells. This means that the wells are separated from one another, and therefore we can consider the eigenvalues and eigenfunctions in each well separately, up to an exponentially small error. We will do this in greater generality in subsection 6.1.

By the Carleman estimate, the eigenfunctions do not vanish in between the wells. In subsection 6.2, we will consider the interaction between the wells. In subsection 6.3, we will return to the one-dimensional symmetric double-well potential.

6.1 Multiple single-well potentials

We will consider a potential V with N wells, and approximate its low-lying eigenvalues and their corresponding eigenfunctions with the eigenvalues and eigenfunctions of multiple single-well potentials $V_j(\nu, b^*)$ where $\nu > 0$ and $b^* > 0$ are small.

Definition 6.1. *(Potential with multiple wells) A potential $V \in S(m_{k,0})$ is said to have N potential wells if:*

(i) There are $b > 0$, $R > 0$ such that the symbol $p - b \in S(m_{k,2})$ is elliptic for all $|x| \geq R$,

(ii) $V : \mathbb{R}^n \to [0, \infty)$,

(iii) There are distinct $x_1, \ldots, x_N \in \mathbb{R}^n$ such that $V(x) = 0 \iff x = x_j$ for some $1 \leq j \leq N$,

(iv) $\partial^2 V(x_j)$ is nonsingular for all $1 \leq j \leq N$.

Now consider $\mathbb{R}^n$ equiped with the Agmon-metric d_V. Let $\nu > 0$ be small enough such that the sets $B_V(x_j, 2\nu)$, $1 \leq j \leq N$ are all disjoint. Let $b^* > 0$ be small enough such that $\{x \in \mathbb{R}^n \mid V(x) \leq b^*\}$ has N connected components, each of which is contained in some $B_V(x_j, \nu)$.

For all $1 \leq j \leq N$, we can define $\vartheta_j \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq \vartheta_j \leq 1$, $\vartheta_j \equiv 1$ on $\{x \in \mathbb{R}^n \mid V(x) \leq b^*\} \cap B_V(x_j, \nu)$, and $\operatorname{Supp}(\vartheta_j) \subseteq B_V(x_j, \nu)$. Then we can define the single-well potentials V_j by

$$V_j(x) := V(x)\left(1 - \sum_{k \neq j} \vartheta_k(x)\right) + b^* \sum_{k \neq j} \vartheta_k(x). \tag{6.1}$$

It should be noted that for all $1 \leq j \leq N$, we have $V_j(x) = 0 \iff x = x_j$, and $V_j > b^*$ outside of $B_V(x_j, \nu)$.

The number of eigenvalues of $P(h) = -h^2\Delta + V(x)$ and $P_j(h) := -h^2\Delta + V_j(x)$ in the interval $[a, b]$ is estimated by Weyl's law.

Theorem 6.2. *(Weyl's law) Let $a < b$ and let $V \in S(m_{k,0})$ for some $k \in \mathbb{N}$. If $p - b \in S(m_{k,2})$ is elliptic for $|x| \geq R$ for some sufficiently large $R > 0$, then the number of eigenvalues between a and b is*

$$\#\{E(h) \mid a \leq E(h) \leq b\} = \frac{1}{(2\pi h)^n}\left(\left|\{(x,\xi) \in \mathbb{R}^{2n} \mid a \leq p(x,\xi) \leq b\}\right| + o(1)\right)$$

as $h \to 0$, where $\left|\{(x,\xi) \in \mathbb{R}^{2n} \mid a \leq p(x,\xi) \leq b\}\right|$ is the volume in $\mathbb{R}^{2n}$.

Remark 6.3. *The notation $o(1)$ means that, for every $\epsilon > 0$, there is a $h_0(\epsilon) > 0$ such that for all $0 < h \leq h_0(\epsilon)$, we have*

$$\left| \#\{E(h) \mid a \leq E(h) \leq b\} - \frac{1}{(2\pi h)^n} \left|\{(x,\xi) \in \mathbb{R}^{2n} \mid a \leq p(x,\xi) \leq b\}\right| \right| \leq \epsilon.$$

We are interested in the lowest lying eigenvalues, so we will consider the case $a = 0$ and $0 < b(h) < b^*$ such that $b(h) \to 0$ as $h \to 0$. Let $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_M < b$ be the eigenvalues of $P(h)$ in the interval $[0, b]$ and let $0 < \mu_{j,1} \leq \mu_{j,2} \leq \ldots \leq \mu_{j,m_j} < b$ be the eigenvalues of $P_j(h)$ in the interval $[0, b]$, where $1 \leq j \leq N$. Let Ω_k be eigenfunction corresponding to λ_k, $1 \leq k \leq M$, and $\eta_{j,k}$ the eigenfunction corresponding to $\mu_{j,k}$, $1 \leq k \leq m_j$. In case an eigenvalue is degenerate, we will count it multiple times and take the eigenfunctions to be orthonormal.

Let for all $1 \leq j \leq N$, $\rho_j \in C_c^\infty(\mathbb{R}^n)$ such that $0 \leq \rho_j \leq 1$, $\rho_j \equiv 1$ on $B_V(x_j, \nu)$, and $\mathrm{Supp}(\rho_j) \subseteq B_V(x_j, 2\nu)$. Define χ_j by $\chi_j(x) := 1 - \sum_{k \neq j} \rho_k(x)$. Then we can define for all $1 \leq j \leq N$, $1 \leq k \leq m_j$,

$$\psi_{j,k} := \chi_j \eta_{j,k}. \tag{6.2}$$

Let E_j be the space spanned by the $\psi_{j,k}$, and let $E := \bigoplus_j E_j$ be their direct sum. Let F be the space spanned by the Ω_j. We want to show that E and F are exponentially close as $h \to 0$.

Definition 6.4. *(Distance between subspaces) Let H be a Hilbert space and let E, F be subspaces. Let π_E and π_F be the projections onto E and F, respectively. Then the non-symmetric distance between E and F is defined as*

$$\vec{d}(E,F) := \|\pi_E - \pi_E \pi_F\| = \|\pi_E - \pi_F \pi_E\|. \tag{6.3}$$

Lemma 6.5. *(Properties of $\vec{d}(\cdot,\cdot)$) Let H be a Hilbert space, and let E, F, G be closed subspaces. Then*

(i) $\vec{d}(E,F) = 0 \Longleftrightarrow E \subseteq F$.

(ii) $\vec{d}(E,G) \leq \vec{d}(E,F) + \vec{d}(F,G)$.

(iii) If $\vec{d}(E,F) < 1$, then $\pi_F|_E : E \to F$ is injective and $\pi_E|_F : F \to E$ is surjective.

(iv) If $\vec{d}(E,F) < 1$ and $\vec{d}(F,E) < 1$, then $\vec{d}(E,F) = \vec{d}(F,E)$.

The following proposition will help us estimate the distance between two subspaces of $L^2(\mathbb{R}^n)$, one of which is the span of eigenfunctions of some operator.

Proposition 6.6. *Let H be a Hilbert space, $D(A) \subseteq H$, $A : D(A) \to H$ a self-adjoint operator. Let $a < b$ and $\epsilon > 0$, and let $\psi_1, \ldots, \psi_M \in D(A)$ be linearly independent such that there are $\lambda_1, \ldots, \lambda_M \in [a,b]$ and $r_1, \ldots, r_M$ with $\|r_k\| \leq \epsilon$ such that*

$$A\psi_k = \lambda_k \psi_k + r_k \tag{6.4}$$

for all $1 \leq k \leq M$. Assume also that there is some $\alpha > 0$ such that

$$\mathit{Spectrum}(A) \cap ((a - 2\alpha, a) \cup (b, b + 2\alpha)) = \emptyset.$$

Finally, let E be the span of the ψ_k, let F be the span of the eigenvectors of A with their corresponding eigenvalue in $[a,b]$, and let λ_S^{min} be the lowest eigenvalue of the matrix $S := (\langle \psi_j, \psi_k \rangle)$. Then

$$\vec{d}(E,F) \leq \frac{M^{1/2}\epsilon}{\alpha(\lambda_S^{min})^{1/2}}. \tag{6.5}$$

Proof. It is a well-known result from spectral theory that

$$\pi_F = \frac{1}{2\pi i} \int_\gamma d\lambda \left[(A - \lambda)^{-1}\right],$$

where γ is some contour around of spectrum$(A) \cap [a,b]$ that does not intersect spectrum(A). We have for all $\lambda \notin$ spectrum(A) that

$$\begin{aligned}\psi_k &= (A-\lambda)^{-1}(A-\lambda)\psi_k = (A-\lambda)^{-1}((\lambda_k-\lambda)\psi_k + r_k)\\ &= (\lambda_k-\lambda)(A-\lambda)^{-1}\psi_k + (A-\lambda)^{-1}r_k,\end{aligned}$$

hence $(A-\lambda)^{-1}\psi_k = (\lambda_k-\lambda)^{-1}\psi_k - (\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k$. Let $R>0$ and let $\gamma = \gamma_R$ be the oriented boundary of $[a-\alpha, b+\alpha] \times i[-R,R]$. By assumption, this boundary does not contain any elements of the spectrum of A. Then

$$\begin{aligned}\pi_F\psi_k &= \frac{1}{2\pi i}\int_{\gamma_R} d\lambda \left[(\lambda_k-\lambda)^{-1}\psi_k - (\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k\right]\\ &= \psi_k - \frac{1}{2\pi i}\int_{\gamma_R} d\lambda \left[(\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k\right]\end{aligned}$$

This last integral tends to

$$\frac{1}{2\pi i}\int_{b+\alpha-iR}^{b+\alpha+iR} d\lambda \left[(\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k\right] - \frac{1}{2\pi i}\int_{a-\alpha-iR}^{a-\alpha+iR} d\lambda \left[(\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k\right]$$

as $R\to\infty$. Setting $\lambda = a-\alpha+ti$ or $\lambda = b+\alpha+ti$ we obtain

$$\|(\lambda_k-\lambda)^{-1}(A-\lambda)^{-1}r_k\| \leq \frac{\epsilon}{\alpha^2+t^2}.$$

Hence $\|\pi_F\psi_k - \psi_k\| \leq \frac{\epsilon}{\pi}\int_{\mathbb{R}} dt\left[\frac{1}{\alpha^2+t^2}\right] = \frac{\epsilon}{\alpha}$. Now let $u \in E$, then there is some $\mu \in \mathbb{C}^M$ such that $u = \sum_{k=1}^M \mu_k\psi_k$. Then $\|u\|^2 = \langle \mu, S\mu\rangle \geq \lambda_S^{\min}\|\mu\|^2$ and $\|\mu\|^2 = \sum_{k,l=1}^M |\mu_k||\mu_l| \leq M\sum_{k=1}^M |\mu_k|^2$. Combining everything, we obtain

$$\|\pi_F u - u\| = \sum_{k=1}^M |\mu_k|\|\pi_F\psi_k - \psi_k\| \leq M^{1/2}\|\mu\|\frac{\epsilon}{\alpha} \leq \frac{M^{1/2}\epsilon}{\alpha(\lambda_S^{\min})^{1/2}}\|u\|. \qquad \square$$

In light of theorem 5.11, we can expect the constant δ to be smaller than the Agmon-distance between the wells. Define for all $0 < b \leq b^*$

$$\delta_b := \min_{j,k} d_{V-b}(x_j, x_k). \tag{6.6}$$

Theorem 6.7. *Let E_j be the space spanned by $\psi_{j,k}$, $1 \leq k \leq m_j$, let $E = \bigoplus_j E_j$, and let F be the space spanned by Ω_k, $1 \leq k \leq M$. Then there is a sufficiently small $h_0 > 0$ such that for all $0 < h \leq h_0$ and all $\delta < \delta_0 - 3\nu$ that*

$$\vec{d}(E,F) = \vec{d}(F,E) = O(e^{-\delta/h}) \tag{6.7}$$

as $h \to 0$. Moreover, there is a bijection $B : \{\lambda_k\}_{1\leq j\leq M} \longrightarrow \{\mu_{j,k}\}_{1\leq j\leq N, 1\leq k\leq m_j}$ such that

$$B(\lambda_k) - \lambda_k = O(e^{-\delta/h}) \tag{6.8}$$

as $h \to 0$ for all $1 \leq k \leq M$.

Proof. We have

$$\begin{aligned}P(h)\psi_{j,k} &= P_j(h)\psi_{j,k} + (V - V_j)\psi_{j,k}\\ &= P_j(h)\psi_{j,k}\\ &= \chi_j P_j(h)\eta_{j,k} + [P_j(h), \chi_j]\eta_{j,k}\\ &= \mu_{j,k}\psi_{j,k} - h^2\left(\eta_{j,k}\Delta\chi_j + 2\langle\partial\chi_j, \partial\eta_{j,k}\rangle_{\mathbb{R}^n}\right)\end{aligned}$$

Now let $\delta < \delta_0 - 3\nu$ and define for $\epsilon > 0$ and a sufficiently large $R > 0$ the sets

$$\begin{aligned}U &:= \bigcup_{k\neq j} B_V(x_k, 2\nu),\\ U_\epsilon &:= B_V(U,\epsilon),\\ W &:= \left(\mathbb{R}^n \backslash \overline{B_V(x_j,\nu)}\right) \cap B_V(0,R).\end{aligned}$$

Note that $\text{Supp}(\partial\chi_j) \subset U \subset\subset U_\epsilon \subset\subset W \subset\subset \{x \in \mathbb{R}^n \mid V(x) > \mu_{j,k}\}$. If ϵ is sufficiently small, we have $\delta < \delta_0 - 3\nu - \epsilon \leq d_V(U_\epsilon, \partial W)$. Then if h is sufficiently small, we obtain $\delta < d_{V-\mu_{j,k}}(U_\epsilon, \partial W)$. Hence by the Agmon-Lithner estimate, we obtain that

$$\|\eta_{j,k}\|_{L^2(\text{Supp}(\partial\chi_j))} \leq \|\eta_{j,k}\|_{L^2(U_\epsilon)} = O(e^{-\delta/h})$$

and

$$\|\partial\eta_{j,k}\|_{L^2(\text{Supp}(\partial\chi_j))} \leq \|\eta_{j,k}\|_{H^2_h(U)} \leq \|\eta_{j,k}\|_{L^2(U_\epsilon)} = O(e^{-\delta/h})$$

as $h \to 0$, where we used proposition 5.7.

Hence $P(h)\psi_{j,k} = \mu_{j,k}\psi_{j,k} + O(e^{-\delta/h})$ as $h \to 0$. Similarly, we obtain $\langle\psi_{j,k}, \psi_{j',k'}\rangle = \delta_{(j,k),(j',k')} + O(e^{-\delta/h})$ as $h \to 0$.

Now we want to use proposition 6.6. We set $A = P(h)$, $\psi_k = \psi_{j,k}$, $a = 0$, $b = b$, $\lambda_k = \mu_{j,k}$. Let $\epsilon' > 0$ be small enough so that $\delta + 2\epsilon' < \delta_0 - 3\nu$ and set $\epsilon = O(e^{-(\delta+2\epsilon')/h})$, $\alpha = e^{-\epsilon'/h}$. By Weyl's law we have $\text{Spectrum}(P(h)) \cap (b, b + 2\alpha) = \emptyset$ and $M^{1/2} = O(e^{\epsilon'/h})$ if h is sufficiently small. Since, $\langle\psi_{j,k}, \psi_{j',k'}\rangle = \delta_{(j,k),(j',k')} + O(e^{-\delta/h})$, we have $\lambda_S^{\min} > 1/2$. Then $\vec{d}(E, F) = O(e^{-\delta/h})$.

Now we need to show that $\vec{d}(F, E) < 1$, because then we have $\vec{d}(F, E) = \vec{d}(E, F)$. Recall that $\rho_j \equiv 1$ on $B_V(x_j, \nu)$ and that $\text{Supp}(\rho_j) \subset B_V(x_j, 2\nu)$. Note in particular, that $V \equiv V_j$ on $\text{Supp}(\rho_j)$. Define also

$$\rho_0 := 1 - \sum_{j=1}^{N} \rho_j, \tag{6.9}$$

and note that $\rho_0\Omega_k = O_{L^2(\mathbb{R}^n)}(e^{-\epsilon/h})$ as $h \to 0$ for some $\epsilon > 0$. Claim: for all $1 \leq j \leq N$ there are $a_{j,l} \in \mathbb{C}$, $1 \leq l \leq m_j$, such that

$$\rho_j\Omega_k = \sum_{l=1}^{m_j} a_{j,l}\eta_{j,l} + O_{L^2(\mathbb{R}^n)}(e^{-\epsilon/h}) \tag{6.10}$$

as $h \to 0$ for some constant $\epsilon > 0$. If this claim holds, then we also have

$$\rho_j\Omega_k = \sum_{l=1}^{m_j} a_{j,l}\psi_{j,l} + O_{L^2(\mathbb{R}^n)}(e^{-\epsilon/h}) \tag{6.11}$$

as $h \to 0$ for some constant $\epsilon > 0$. Then we obtain

$$\Omega_k = \sum_{j=0}^{N} \rho_j\Omega_k = \sum_{j=1}^{N}\sum_{l=1}^{m_j} a_{j,l}\psi_{j,l} + O_{L^2(\mathbb{R}^n)}(e^{-\epsilon/h}). \tag{6.12}$$

But the $\{\Omega_k\}_{1\leq k\leq M}$ is a basis of F. So $\vec{d}(F, E) = \|(I - \pi_E)\pi_F\| = O(e^{-\epsilon/h})$ as $h \to 0$. So if h is sufficiently small, we obtain $\vec{d}(F, E) < 1$ as desired.

Now, to prove the claim, note that

$$\begin{aligned} P_j(h)(\rho_j\Omega_k) &= P(h)(\rho_j\Omega_k) && (6.13)\\ &= \lambda_k\rho_j\Omega_k + [P(h), \rho_j]\Omega_k && (6.14)\\ &= \lambda_k\rho_j\Omega_k + O_{L^2(\mathbb{R}^n)}(e^{-4\epsilon/h}) && (6.15)\end{aligned}$$

as $h \to 0$ for some $\epsilon > 0$. Define the following subspaces of $L^2(\mathbb{R}^n)$: let $F_{j,k}$ be the span of $\rho_j\Omega_k$, and let $\tilde{E}_j$ be the span of $\eta_{j,l}$, $1 \leq l \leq m_j$. We may assume without loss of generality that $\|\rho_j\Omega_k\| > e^{-\epsilon/h}$ (otherwise we could pick $a_{j,l} := 0$). Now we will apply proposition 6.6 with $A = P_j(h)$, $\alpha = e^{-\epsilon/h}$, $\lambda_S^{\min} = \|\rho_j\Omega_k\| > e^{-\epsilon/h}$, and $m_j^{1/2} = O(e^{\epsilon/h})$. Then we obtain

$$\vec{d}(F_{j,l}, \tilde{E}_j) \leq C\frac{e^{\epsilon/h}e^{-4\epsilon/h}}{e^{-\epsilon/h}e^{-\epsilon/h}} = O(e^{-\epsilon/h}). \tag{6.16}$$

But then $\rho_j \Omega_k = \pi_{\tilde{E}_j}(\rho_j \Omega_k) + O_{L^2(\mathbb{R}^n)}(e^{-\epsilon/h})$ as desired.

Finally, we need to show there is a bijection $B : \{\lambda_k\}_{1\leq j\leq M} \longrightarrow \{\mu_{j,k}\}_{1\leq j\leq N, 1\leq k\leq m_j}$ such that for all $\delta < \delta_0 - 3\nu$, $1 \leq k \leq M$, we have $B(\lambda_k) - \lambda_k = O(e^{-\delta/h})$ as $h \to 0$. Since $\vec{d}(E,F) = \vec{d}(F,E) < 1$ if h is sufficiently small, there is a homeomorphism between E and F, and so $M = \sum_{j=1}^N m_j$.

Now let $\delta' < \delta < \delta_0 - 3\nu$ and divide the interval $[0,b]$ in smaller intervals of width $2e^{-\delta'/h}$, i.e. we define for $i \in \mathbb{N}$ the interval $I_i := [2ie^{-\delta'/h}, 2(i+1)e^{-\delta'/h}]$. Without loss of generality, we may assume that if h is sufficiently small, we have

$$I_i \cap \{\lambda_k\}_{1\leq k\leq M} \neq \emptyset \implies I_{i+1} \cap \{\lambda_k\}_{1\leq k\leq M} = \emptyset.$$

Then we can again apply proposition 6.6 similar to the proof of $\vec{d}(E,F) = O(e^{-\delta/h})$, but now with the interval I_i instead of $[0,b]$. In this case, since $\alpha = e^{-\delta'/h}$, we obtain $\vec{d}(E,F) = O(e^{-(\delta-\delta')/h})$. Since $\delta' < \delta$, we have $\vec{d}(E,F) < 1$ if h is sufficiently small. Then $\pi_F\, |_E \colon E \to F$ is injective, so the interval I_i contains at least as many λ_k as $\mu_{j,l}$. But we already have $M = m_1 + \ldots m_N$, hence the interval I_i must in fact contain as many λ_k as $\mu_{j,l}$. So we can define a bijection B such that $B(\lambda_k) - \lambda_k = O(e^{-\delta'/h})$ as $h \to 0$. □

Notation 6.8. *($\tilde{O}$-notation) Let $\delta_0 > 0$, then the notation*

$$A(\nu) = \tilde{O}(e^{-\delta_0/h})$$

means that for all $\delta < \delta_0$, there is a sufficiently small $\nu > 0$ such that $A(\nu) = O(e^{-\delta/h})$ as $h \to 0$.

6.2 The matrix representation of the Schrödinger operator

As theorem 6.7 shows, we can consider each well separately up to some exponentially small error. However, due to quantum tunneling, there will still be some interaction between the wells. In this subsection, we will discuss this interaction. But first, we will prove a few facts about the projection π_F.

Proposition 6.9. *The following statements hold:*

(i) $\pi_F \psi_{j,k} = \psi_{j,k} + \tilde{O}(e^{-\delta_0/h})$,

(ii) π_F *commutes with* $P(h)$,

(iii) $\langle \pi_F \psi_{j,k}, \pi_F \psi_{j',k'} \rangle = \langle \psi_{j,k}, \psi_{j',k'} \rangle - \langle \pi_F \psi_{j,k} - \psi_{j,k}, \pi_F \psi_{j',k'} - \psi_{j',k'} \rangle$,

(iv) $\langle \pi_F \psi_{j,k}, P(h) \pi_F \psi_{j',k'} \rangle = \langle \psi_{j,k}, P(h) \psi_{j',k'} \rangle - \langle \pi_F \psi_{j,k} - \psi_{j,k}, P(h)(\pi_F \psi_{j',k'} - \psi_{j',k'}) \rangle$.

Proof. (i) Let $\delta < \delta_0$, then there is a sufficiently small $\nu > 0$ such that $\delta < \delta_0 - 3\nu$. By theorem 6.7, we have $\|(\pi_F - I)\pi_E\| = \vec{d}(E,F) = O(e^{-\delta/h})$. But then

$$\|\pi_F \psi_{j,k} - \psi_{j,k}\|_{L^2(\mathbb{R}^n)} = \|(\pi_F - I)\pi_E \psi_{j,k}\|_{L^2(\mathbb{R}^n)} = O(e^{-\delta/h}).$$

(ii) The eigenfunctions $\{\Omega_k\}_{k\in\mathbb{N}}$ of $P(h)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$. If $1 \leq k \leq M$, we have $\pi_F \Omega_k = \Omega_k$. Otherwise, we have $\pi_F \Omega_k = 0$. Hence π_F commutes with $P(h)$.

(iii) Note that $I - \pi_F$ is an orthogonal projection onto $F^\perp$. So $I - \pi_F$ is idempotent and self-adjoint. Now we can calculate:

$$\begin{aligned}\langle (\pi_F - I)\psi_{j,k}, (\pi_F - I)\psi_{j',k'} \rangle &= \langle (I - \pi_F)\psi_{j,k}, (I - \pi_F)\psi_{j',k'} \rangle \\ &= \langle (I - \pi_F)\psi_{j,k}, \psi_{j',k'} \rangle \\ &= \langle \psi_{j,k}, \psi_{j',k'} \rangle - \langle \pi_F \psi_{j,k}, \pi_F \psi_{j',k'} \rangle.\end{aligned}$$

(iv) This follows trivially from (ii) and (iii). □

Define for $1 \leq j \leq N$, $1 \leq j \leq m_j$,

$$\varphi_{j,k} := \pi_F \psi_{j,k}. \tag{6.17}$$

By theorem 6.7 and proposition 6.9, we obtain that $\{\varphi_{j,k}\}$ is a basis of F, and the interaction between the wells is characterised by the $M \times M$-matrix $(\langle \varphi_{j,k}, P(h)\varphi_{j',k'}\rangle)$. Recall that

$$\varphi_{j,k} - \psi_{j,k} = \tilde{O}(e^{-\delta_0/h})$$

and that

$$P(h)\psi_{j,k} = \mu_{j,k}\psi_{j,k} + r_{j,k},$$

where

$$r_{j,k} := [P(h), \chi_j]\eta_{j,k} = \tilde{O}(e^{-\delta_0/h}).$$

Then we have

$$\begin{aligned} P(h)(\varphi_{j,k} - \psi_{j,k}) &= (\pi_F - I)P(h)\psi_{j,k} \\ &= (\pi_F - I)(\mu_{j,k}\psi_{j,k} + r_{j,k}) \\ &= \mu_{j,k}(\varphi_{j,k} - \psi_{j,k}) + (\pi_F - I)r_{j,k}. \end{aligned}$$

So $P(h)(\varphi_{j,k} - \psi_{j,k}) = O(e^{-\delta/h})$, and so $\langle \varphi_{j,k} - \psi_{j,k}, P(h)(\varphi_{j,k} - \psi_{j,k})\rangle = \tilde{O}(e^{-2\delta_0/h})$. Moreover, we have

$$\begin{aligned} \langle \psi_{j,k}, P(h)\psi_{j',k'}\rangle &= \frac{1}{2}\left(\langle \psi_{j,k}, P(h)\psi_{j',k'}\rangle + \langle P(h)\psi_{j,k}, \psi_{j',k'}\rangle\right) \\ &= \frac{1}{2}\left(\langle \psi_{j,k}, \mu_{j',k'}\psi_{j',k'} + r_{j',k'}\rangle + \langle \mu_{j,k}\psi_{j,k} + r_{j,k}, \psi_{j',k'}\rangle\right) \\ &= \frac{\mu_{j,k} + \mu_{j',k'}}{2}\langle \psi_{j,k}, \psi_{j',k'}\rangle + \frac{1}{2}\left(\langle \psi_{j,k}, r_{j',k'}\rangle + \langle r_{j,k}, \psi_{j',k'}\rangle\right), \end{aligned}$$

and

$$\begin{aligned} \langle \psi_{j,k}, r_{j',k'}\rangle &= \langle \chi_j\eta_{j,k}, [P(h), \chi_{j'}]\eta_{j',k'}\rangle \\ &= h^2\sum_{i=1}^n \left[-\langle \chi_j\eta_{j,k}, \partial_i^2(\chi_{j'})\eta_{j',k'}\rangle - 2\langle \chi_j\eta_{j,k}, (\partial_i\chi_{j'})\partial_i\eta_{j',k'}\rangle\right] \\ &= h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[-\chi_j(x)\overline{\eta_{j,k}(x)}(\partial_i^2\chi_{j'})(x)\eta_{j',k'}(x) - 2\chi_j(x)\overline{\eta_{j,k}(x)}(\partial_i\chi_{j'})(x)(\partial_i\eta_{j',k'})(x)\right] \\ &= h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[\partial_i(\chi_j\overline{\eta_{j,k}}\eta_{j',k'})(x)(\partial_i\chi_{j'})(x) - 2\chi_j(x)\overline{\eta_{j,k}(x)}(\partial_i\chi_{j'})(x)(\partial_i\eta_{j',k'})(x)\right] \\ &= h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[\partial_i(\chi_j\overline{\eta_{j,k}}\eta_{j',k'})(x)(\partial_i\chi_{j'})(x) - 2\chi_j(x)\overline{\eta_{j,k}(x)}(\partial_i\chi_{j'})(x)(\partial_i\eta_{j',k'})(x)\right] \\ &= h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[\chi_j(x)\left(\overline{\partial_i\eta_{j,k}(x)}\eta_{j',k'}(x) - \overline{\eta_{j,k}(x)}(\partial_i\eta_{j',k'})(x)\right)(\partial_i\chi_{j'})(x)\right] \\ &\quad + h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[(\partial_i\chi_j)(x)\overline{\eta_{j,k}(x)}\eta_{j',k'}(x)(\partial_i\chi_{j'})(x)\right]. \end{aligned}$$

But $\eta_{j,k} = \tilde{O}(e^{-\delta_0/h})$ on $\operatorname{Supp}(\partial_i\chi_j)$, hence the second term is $\tilde{O}(e^{-2\delta_0/h})$. Now define

$$w_{(j,k),(j',k')} := h^2\sum_{i=1}^n \int_{\mathbb{R}^n} dx \left[\chi_j(x)\left(\overline{\partial_i\eta_{j,k}(x)}\eta_{j',k'}(x) - \overline{\eta_{j,k}(x)}(\partial_i\eta_{j',k'})(x)\right)(\partial_i\chi_{j'})(x)\right], \tag{6.18}$$

$$W_{(j,k),(j',k')} := \frac{1}{2}\left(w_{(j,k),(j',k')} + w_{(j',k'),(j,k)}\right). \tag{6.19}$$

Putting everything together, we obtain

$$\langle \varphi_{j,k}, P(h)\varphi_{j',k'}\rangle = \frac{1}{2}\left(\mu_{j,k} + \mu_{j',k'}\right)\langle \psi_{j,k}, \psi_{j',k'}\rangle + W_{(j,k),(j',k')} + \tilde{O}(e^{-2\delta_0/h}), \tag{6.20}$$

the matrix of $P|_F(h) : F \to F$ in the basis $\{\varphi_{j,k}\}$. Note that we have $W_{(j,k),(j',k')} = \tilde{O}(e^{-\delta_0/h})$. However, we also have $\langle \psi_{j,k}, \psi_{j',k'}\rangle = \delta_{(j,k),(j',k')} + \tilde{O}(e^{-\delta_0/h})$, so this term contributes to the matrix of $P|_F(h)$ in the same order as $W_{(j,k),(j',k')}$.

This owes to the fact that $\{\varphi_{j,k}\}$ is not orthonormal. Therefore, it is more convenient to write the matrix of $P|_F(h)$ in an orthonormal basis. Define

$$N := (\langle \varphi_{j,k}, \varphi_{j',k'}\rangle) = (\varphi_{1,1} \dots \varphi_{N,m_N})^T(\varphi_{1,1} \dots \varphi_{N,m_N}). \tag{6.21}$$

We have $\langle \varphi_{j,k}, \varphi_{j',k'}\rangle = \langle \psi_{j,k}, \psi_{j',k'}\rangle - \langle \varphi_{j,k} - \psi_{j,k}, \varphi_{j',k'} - \psi_{j',k'}\rangle = \delta_{(j,k),(j',k')} + \tilde{O}(e^{-\delta_0/h}) + \tilde{O}(e^{-2\delta_0/h})$, so

$$N = I + \tilde{O}(e^{-\delta_0/h}), \text{ and} \tag{6.22}$$

$$N^{-1/2} = I + \tilde{O}(e^{-\delta_0/h}). \tag{6.23}$$

Then we can define the functions $e_{j,k}$ by

$$(e_{1,1} \dots e_{N,m_N}) := (\varphi_{1,1} \dots \varphi_{N,m_N})N^{-1/2}. \tag{6.24}$$

Then

$$\begin{aligned}(e_{1,1} \dots e_{N,m_N})^T(e_{1,1} \dots e_{N,m_N}) &= N^{-1/2}(\varphi_{1,1} \dots \varphi_{N,m_N})^T(\varphi_{1,1} \dots \varphi_{N,m_N})N^{-1/2} \\ &= N^{-1/2}NN^{-1/2} = I,\end{aligned}$$

so the basis $\{e_{j,k}\}$ is indeed orthonormal. Calculating the matrix of $P|_F(h)$ in this basis gives

$$\begin{aligned}&(e_{1,1} \dots e_{N,m_N})^T P(h)(e_{1,1} \dots e_{N,m_N}) \\ &\quad = N^{-1/2}(\varphi_{1,1} \dots \varphi_{N,m_N})^T P(h)(\varphi_{1,1} \dots \varphi_{N,m_N})N^{-1/2} \\ &\quad = \mathrm{diag}(\mu_{1,1}, \dots, \mu_{N,m_N}) + (I + O(e^{-\delta/h}))(W_{(j,k),(j',k')})(I + O(e^{-\delta/h})) + \tilde{O}(e^{-2\delta_0/h}) \\ &\quad = \mathrm{diag}(\mu_{1,1}, \dots, \mu_{N,m_N}) + (W_{(j,k),(j',k')}) + \tilde{O}(e^{-2\delta_0/h}).\end{aligned}$$

6.3 The one-dimensional symmetric double-well potential

We will now apply the results of the previous subsection to a one-dimensional symmetric double-well potential, i.e. $n = 1$, $V(x) = V(-x)$ for all $x \in \mathbb{R}$, and V has two wells $x_A, x_B \in \mathbb{R}$.

Let $\delta < \delta_0$ and let $\nu > 0$ be small enough such that $\delta < \delta_0 - 3\nu$. Then we can choose $b^* > 0$ small enough such that $\{x \in \mathbb{R} \mid V(x) \leq b^*\}$ has two connected components and is contained in $B_V(x_A, \nu) \cup B_V(x_B, \nu)$. Let $\theta_A \in C_c^\infty(\mathbb{R})$ such that $0 \leq \theta_A \leq 1$, $\theta_A \equiv 1$ on $\{x \in \mathbb{R} \mid V(x) \leq b^*\} \cap B_V(x_A, \nu)$, and $\mathrm{Supp}(\theta_A) \subseteq B_V(x_A, \nu)$. Define $\theta_B \in C_c^\infty(\mathbb{R})$ by $\theta_B(x) := \theta_A(-x)$.

Then we can define the single-well potentials V_A and V_B by

$$V_A(x) := V(x)(1 - \theta_B(x)) + b^*\theta_B(x), \tag{6.25}$$

$$V_B(x) := V_A(-x). \tag{6.26}$$

Let $0 < b(h) < b^*$ such that $P(h) := -h^2\partial_x^2 + V(x)$ has two eigenvalues in $[0, b]$. We will denote these eigenvalues by E_+ and E_-, and their respective eigenfunctions Ω_+ and Ω_-. By symmetry, we know that $P_A(h)$ and $P_B(h)$ each have one eigenvalue in $[0, b]$, and that $\mu_A = \mu_B =: \mu$ with eigenfunctions η_A and η_B such that $\eta_B(x) := \eta_A(-x)$.

Let $\rho_A \in C_c^\infty(\mathbb{R})$ such that $0 \leq \rho_A \leq 1$, $\rho_A \equiv 1$ on $B_V(x_A, \nu)$, and $\mathrm{Supp}(\rho_A) \subseteq B_V(x_A, 2\nu)$ and define $\rho_B \in C_c^\infty(\mathbb{R})$ by $\rho_B(x) := \rho_A(-x)$. Let

$$\chi_A := 1 - \rho_B, \qquad \chi_B := 1 - \rho_A, \tag{6.27}$$

$$\psi_A := \chi_A \eta_A, \qquad \psi_B := \chi_B \eta_B. \tag{6.28}$$

Let $F := \mathrm{Span}(\Omega_-, \Omega_+)$, and define

$$\varphi_A := \pi_F \psi_A, \tag{6.29}$$

$$\varphi_B := \pi_F \psi_B. \tag{6.30}$$

Let

$$N := \begin{pmatrix} \varphi_A \\ \varphi_B \end{pmatrix} \begin{pmatrix} \varphi_A & \varphi_B \end{pmatrix} = \begin{pmatrix} \langle \varphi_A, \varphi_A \rangle & \langle \varphi_A, \varphi_B \rangle \\ \langle \varphi_B, \varphi_A \rangle & \langle \varphi_B, \varphi_B \rangle \end{pmatrix}, \tag{6.31}$$

then we can finally define the orthonormal basis $\{e_A, e_B\}$ of F by

$$\begin{pmatrix} e_A & e_B \end{pmatrix} = \begin{pmatrix} \varphi_A & \varphi_B \end{pmatrix} N^{-1/2}. \tag{6.32}$$

We have $W_{A,A} = W_{B,B} = 0$ and $W_{A,B} = W_{B,A} =: \beta$. Then the matrix of $P|_F(h)$ in the basis $\{e_A, e_B\}$ is

$$\begin{pmatrix} e_A \\ e_B \end{pmatrix} P(h) \begin{pmatrix} e_A & e_B \end{pmatrix} = \begin{pmatrix} \mu & 0 \\ 0 & \mu \end{pmatrix} + \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix} + \tilde{O}(e^{-2\delta_0/h}) \tag{6.33}$$

$$= \begin{pmatrix} \mu + r_1 & \beta + r_2 \\ \beta + r_2 & \mu + r_1 \end{pmatrix}, \tag{6.34}$$

where $r_1, r_2 = \tilde{O}(e^{-2\delta_0/h})$. The eigenvalues of this matrix are

$$E_\pm = \mu + r_1 \pm |\beta + r_2|, \tag{6.35}$$

$$= \mu \pm \mathrm{sign}(\beta)\beta + \tilde{O}(e^{-2\delta_0/h}), \tag{6.36}$$

and the eigenfunctions are

$$\Omega_\pm = \frac{1}{\sqrt{2}} e_A \pm \mathrm{sign}(\beta) \frac{1}{\sqrt{2}} e_B \tag{6.37}$$

$$= \frac{1}{\sqrt{2}} \eta_A \pm \mathrm{sign}(\beta) \frac{1}{\sqrt{2}} \eta_B + \tilde{O}(e^{-\delta_0/h}). \tag{6.38}$$

So we have found that the lowest two eigenvalues are $\mu + \tilde{O}(e^{-\delta_0/h})$ and $|E_+ - E_-| = 2|\beta| = \tilde{O}(e^{-\delta_0/h})$. Moreover, the eigenfunctions are not localised in one particular well. Both wells contribute equally.

7 Breaking the symmetry

In this section we will again look at the one-dimensional double-well potential V. We will consider a non-negative perturbation $\Delta V \in C_c^\infty(\mathbb{R})$ such that $\overline{\text{Supp}(\Delta V)} \cap \{x_A, x_B\} = \emptyset$. Then we can define the perturbed potential $\tilde{V}$ by

$$\tilde{V} := V + t\Delta V, \tag{7.1}$$

where the parameter $t \in [-1, 1]$ regulates the strength and the sign of the perturbation. We will consider the case where ΔV is not symmetric, and look at the consequences for the lowest two eigenvalues $\tilde{E}_\pm$ of $\tilde{P}(h) := -h^2\Delta + \tilde{V}$ and their respective eigenvectors $\tilde{\Omega}_\pm$.

7.1 Perturbation of the single-well potential

We will first consider the single-well potential $\tilde{V}_j$, $j \in \{A, B\}$. Since $\overline{\text{Supp}(\Delta V)} \cap \{x_A, x_B\} = \emptyset$, we can choose $\tilde{\theta}_j = \theta_j$ and $\tilde{\chi}_j = \chi_j$ when h is sufficiently small, so we can simply set $\tilde{V}_j := V_j + t\Delta V$. Define

$$\tilde{P}_j(h) := -h^2\Delta + \tilde{V}_j, \tag{7.2}$$

and let $\tilde{\mu}_j$ be its lowest eigenvalue with eigenfunction $\tilde{\eta}_j$. Let δ_j be the Agmon-distance between the well x_j and the support of the perturbation ΔV, i.e.

$$\delta_j = d_V(x_j, \text{Supp}(\Delta V)). \tag{7.3}$$

Proposition 7.1. *Let μ and η_j be the lowest eigenvalue and the corresponding eigenfunction of the unperturbed potential, then we have*

$$\tilde{\mu}_j = \mu + t\langle \eta_j, \Delta V \eta_j\rangle + t^2\tilde{O}(e^{-3\delta_j/h}), \tag{7.4}$$

and

$$\tilde{\eta}_j = \eta_j + t\tilde{O}(e^{-\delta_j/h}). \tag{7.5}$$

Proof. Let $r_j := t\Delta V \eta_j$. By the Agmon-Lithner estimate, we have $r_j = t\tilde{O}(e^{-\delta_j/h})$. Then

$$\begin{aligned}\tilde{P}_j(h)\eta_j &= P_j(h)\eta_j + t\Delta V\eta_j \\ &= \mu\eta_j + r_j.\end{aligned}$$

Let E_j be the span of η_j and let $\tilde{E}_j$ be the span of $\tilde{\eta}_j$. Then we obtain by proposition 6.6 that $\vec{d}(\pi_{E_j}, \pi_{\tilde{E}_j}) = t\tilde{O}(e^{-\delta_j/h})$. Then we have

$$1 = \|\eta_j\|^2 = \|\pi_{\tilde{E}_j}\eta_j\|^2 + \|(I - \pi_{\tilde{E}_j})\eta_j\|^2 = \|\pi_{\tilde{E}_j}\eta_j\|^2 + t^2\tilde{O}(e^{-2\delta_j/h}),$$

so we obtain $\|\pi_{\tilde{E}_j}\eta_j\|^{-1} = 1 + t^2\tilde{O}(e^{-2\delta_j/h})$ by taking the Taylor expansion of the function $f(x) = x^{-1/2}$ and applying it to $\|\pi_{\tilde{E}_j}\eta_j\|^2$. But $\tilde{E}_j$ is a one-dimensional space, so we have

$$\begin{aligned}\tilde{\eta}_j &= \|\pi_{\tilde{E}_j}\eta_j\|^{-1}\pi_{\tilde{E}_j}\eta_j \\ &= \pi_{\tilde{E}_j}\eta_j + t^2\tilde{O}(e^{-2\delta_j/h}) \\ &= \eta_j - (I - \pi_{\tilde{E}_j})\eta_j + t^2\tilde{O}(e^{-2\delta_j/h}) \\ &= \eta_j + t\tilde{O}(e^{-\delta_j/h})\end{aligned}$$

and

$$\begin{aligned}
\tilde{\mu}_j &= \langle \tilde{\eta}_j, \tilde{P}_j(h)\tilde{\eta}_j\rangle \\
&= \|\pi_{\tilde{E}_j}\eta_j\|^{-2}\langle \pi_{\tilde{E}_j}\eta_j, \tilde{P}_j(h)\pi_{\tilde{E}_j}\eta_j\rangle \\
&= \|\pi_{\tilde{E}_j}\eta_j\|^{-2}\langle \pi_{\tilde{E}_j}\eta_j, \pi_{\tilde{E}_j}\tilde{P}_j(h)\eta_j\rangle \\
&= \|\pi_{\tilde{E}_j}\eta_j\|^{-2}\langle \pi_{\tilde{E}_j}\eta_j, \pi_{\tilde{E}_j}(\mu\eta_j + t\Delta V\eta_j)\rangle \\
&= \mu + \|\pi_{\tilde{E}_j}\eta_j\|^{-2}\langle \pi_{\tilde{E}_j}\eta_j, t\Delta V\eta_j\rangle \\
&= \mu + \|\pi_{\tilde{E}_j}\eta_j\|^{-2}\langle \eta_j - (I-\pi_{\tilde{E}_j})\eta_j, t\Delta V\eta_j\rangle \\
&= \mu + \left(1 + t^2\tilde{O}(e^{-2\delta_j/h})\right)\left(t\langle \eta_j, \Delta V\eta_j\rangle + t^2\tilde{O}(e^{-3\delta_j/h})\right) \\
&= \mu + t\langle \eta_j, \Delta V\eta_j\rangle + t^2\tilde{O}(e^{-3\delta_j/h}),
\end{aligned}$$

where we used that

$$\begin{aligned}
|t\langle \eta_j, \Delta V\eta_j\rangle| &\le |t|\|\eta_j\|_{L^2(\mathrm{Supp}(\Delta V))}\|\Delta V\eta_j\| \\
&= t\tilde{O}(e^{-2\delta_j/h})
\end{aligned}$$

and

$$\begin{aligned}
|t\langle (I-\pi_{\tilde{E}_j})\eta_j, \Delta V\eta_j\rangle| &\le |t|\|(I-\pi_{\tilde{E}_j})\eta_j\|_{L^2(\mathrm{Supp}(\Delta V))}\|\Delta V\eta_j\| \\
&\le |t|\|(I-\pi_{\tilde{E}_j})\pi_{E_j}\|\|\eta_j\|_{L^2(\mathrm{Supp}(\Delta V))}\|\Delta V\eta_j\| \\
&= t^2\tilde{O}(e^{-3\delta_j/h}).
\end{aligned}$$

□

7.2 Perturbation of the double-well potential

In this subsection, we will consider the two lowest eigenvalues $\tilde{E}_\pm$ and their corresponding eigenfunctions $\tilde{\Omega}_\pm$ of the perturbed one-dimensional symmetric double-well potential $\tilde{V} = V + t\Delta V$. Let $\tilde{F}$ be the space spanned by $\tilde{\Omega}_\pm$. As before, there is an orthonormal basis $\{\tilde{e}_A, \tilde{e}_B\}$ of $\tilde{F}$ such that

$$\begin{pmatrix}\tilde{e}_A \\ \tilde{e}_B\end{pmatrix} \tilde{P}(h) \begin{pmatrix}\tilde{e}_A & \tilde{e}_B\end{pmatrix} = \begin{pmatrix}\tilde{\mu}_A & \tilde{\beta} \\ \tilde{\beta} & \tilde{\mu}_B\end{pmatrix} + \tilde{O}(e^{-2\delta_0/h}),$$

where $\tilde{\beta} := \tilde{W}_{A,B}$. In the previous subsection, we found that

$$\tilde{\mu}_A = \mu + t\langle \eta_A, \Delta V\eta_A\rangle + t^2\tilde{O}(e^{-3\delta_A/h}), \tag{7.6}$$

$$\tilde{\mu}_B = \mu + t\langle \eta_B, \Delta V\eta_B\rangle + t^2\tilde{O}(e^{-3\delta_B/h}). \tag{7.7}$$

Moreover, recall that $\tilde{e}_j = \tilde{\eta}_j + \tilde{O}(e^{-\delta_0/h})$. Then we obtain

$$\tilde{e}_A = \eta_A + t\tilde{O}(e^{-\delta_A/h}) + \tilde{O}(e^{-\delta_0/h}), \tag{7.8}$$

$$\tilde{e}_B = \eta_B + t\tilde{O}(e^{-\delta_B/h}) + \tilde{O}(e^{-\delta_0/h}). \tag{7.9}$$

Now it is only left to estimate $\tilde{\beta} - \beta$.

Proposition 7.2. *We have*

$$\tilde{\beta} = \beta + t\Re(\langle \eta_A, \Delta V\eta_B\rangle) + t\tilde{O}(e^{-(\delta_0+\min(\delta_A,\delta_B))/h}) \tag{7.10}$$

Proof. We have

$$\begin{aligned}
\tilde{w}_{A,B} &= h^2\int_{\mathbb{R}} dx\left[\chi_A(x)\left(\overline{\partial\tilde{\eta}_A(x)}\tilde{\eta}_B(x) - \overline{\tilde{\eta}_A(x)}\partial\tilde{\eta}_B(x)\right)\partial\chi_B(x)\right] \\
&= h^2\langle \chi_A\partial\tilde{\eta}_A, \partial\chi_B\tilde{\eta}_B\rangle - h^2\langle \chi_A\tilde{\eta}_A, \partial\chi_B\partial\tilde{\eta}_B\rangle \\
&= h^2\langle \chi_A\partial\eta_A, \partial\chi_B\eta_B\rangle - h^2\langle \chi_A\eta_A, \partial\chi_B\partial\eta_B\rangle \\
&\quad + h^2\langle \chi_A\partial(\tilde{\eta}_A - \eta_A), \partial\chi_B\tilde{\eta}_B\rangle - h^2\langle \chi_A(\tilde{\eta}_A - \eta_A), \partial\chi_B\partial\tilde{\eta}_B\rangle \\
&\quad + h^2\langle \chi_A\partial\eta_A, \partial\chi_B(\tilde{\eta}_B - \eta_B)\rangle - h^2\langle \chi_A\eta_A, \partial\chi_B\partial(\tilde{\eta}_B - \eta_B)\rangle.
\end{aligned}$$

We will estimate each of these terms separately. Since the terms involving $\tilde{\eta}_B - \eta_B$ cannot be estimated directly, we will first rewrite them by integrating by parts.

- $$\begin{aligned}\langle \chi_A \partial\eta_A, \partial\chi_B(\tilde{\eta}_B - \eta_B)\rangle &= \int_{\mathbb{R}} dx \left[\chi_A(x)\overline{\partial\eta_A(x)}(\tilde{\eta}_B - \eta_B)(x)\partial\chi_B(x)\right] \\ &= -\int_{\mathbb{R}} dx \left[\partial(\chi_A\overline{\partial\eta_A}(\tilde{\eta}_B - \eta_B))(x)\chi_B(x)\right] \\ &= -\langle \partial\chi_A\partial\eta_A, \chi_B(\tilde{\eta}_B - \eta_B)\rangle \\ &\quad - \int_{\mathbb{R}} dx \left[\chi_A(x)\left(\overline{\partial^2\eta_A(x)}(\tilde{\eta}_B - \eta_B)(x) + \overline{\partial\eta_A(x)}\partial(\tilde{\eta}_B - \eta_B)(x)\right)\chi_B(x)\right]\end{aligned}$$
- $$\begin{aligned}-\langle \chi_A\eta_A, \partial\chi_B\partial(\tilde{\eta}_B - \eta_B)\rangle &= -\int_{\mathbb{R}} dx \left[\chi_A(x)\overline{\eta_A(x)}\partial(\tilde{\eta}_B - \eta_B)(x)\partial\chi_B(x)\right] \\ &= \int_{\mathbb{R}} dx \left[\partial(\chi_A\overline{\eta_A}\partial(\tilde{\eta}_B - \eta_B))(x)\chi_B(x)\right] \\ &= \langle \partial\chi_A\eta_A, \chi_B\partial(\tilde{\eta}_B - \eta_B)\rangle \\ &\quad + \int_{\mathbb{R}} dx \left[\chi_A(x)\left(\overline{\partial\eta_A(x)}\partial(\tilde{\eta}_B - \eta_B)(x) + \overline{\eta_A(x)}\partial^2(\tilde{\eta}_B - \eta_B)(x)\right)\chi_B(x)\right]\end{aligned}$$

On $\mathrm{Supp}(\chi_A) \cap \mathrm{Supp}(\chi_B)$, we have $V \equiv V_A \equiv V_B$ and $\tilde{V} \equiv \tilde{V}_A \equiv \tilde{V}_B$. Combined with $-h^2\partial^2 = P(h) - V = \tilde{P}(h) - \tilde{V}$, we get for all $x \in \mathrm{Supp}(\chi_A) \cap \mathrm{Supp}(\chi_B)$ that

$$\begin{aligned}h^2\partial^2(\tilde{\eta}_B - \eta_B)(x) &= h^2\partial^2\tilde{\eta}_B(x) - h^2\partial^2\eta_B(x) \\ &= -(\tilde{P}_B(h) - \tilde{V}_B)\tilde{\eta}_B(x) + (P_B(h) - V_B)\eta_B(x) \\ &= -\tilde{\mu}_B\tilde{\eta}_B(x) + \tilde{V}(x)\tilde{\eta}_B(x) + \mu\eta_B(x) - V(x)\eta_B(x), \\ -h^2\partial^2\eta_A(x) &= (P_A(h) - V_A)\eta_A(x) \\ &= \mu\eta_A(x) - V(x)\eta_A(x).\end{aligned}$$

Hence

$$\begin{aligned}&h^2\left(\overline{\eta_A(x)}\partial^2(\tilde{\eta}_B - \eta_B)(x) - \overline{\partial^2\eta_A(x)}(\tilde{\eta}_B - \eta_B)(x)\right) \\ &\qquad = -(\tilde{\mu}_B - \mu)\overline{\eta_A(x)}\tilde{\eta}_B(x) + (\tilde{V} - V)(x)\overline{\eta_A(x)}\tilde{\eta}_B(x).\end{aligned}$$

Putting it all together, we obtain

$$\begin{aligned}\tilde{w}_{A,B} &= w_{A,B} \\ &\qquad + h^2\langle \chi_A\partial(\tilde{\eta}_A - \eta_A), \partial\chi_B\tilde{\eta}_B\rangle - h^2\langle \chi_A(\tilde{\eta}_A - \eta_A), \partial\chi_B\partial\tilde{\eta}_B\rangle \\ &\qquad + h^2\langle \partial\chi_A\eta_A, \chi_B\partial(\tilde{\eta}_B - \eta_B)\rangle - h^2\langle \partial\chi_A\partial\eta_A, \chi_B(\tilde{\eta}_B - \eta_B)\rangle \\ &\qquad + \langle \chi_A\eta_A, (\tilde{V} - V)\chi_B\tilde{\eta}_B\rangle - (\tilde{\mu}_B - \mu)\langle \chi_A\eta_A, \chi_B\tilde{\eta}_B\rangle \\ &= w_{A,B} + t\langle \eta_A, \Delta V\eta_B\rangle \\ &\qquad + h^2\langle \chi_A\partial(\tilde{\eta}_A - \eta_A), \partial\chi_B\tilde{\eta}_B\rangle - h^2\langle \chi_A(\tilde{\eta}_A - \eta_A), \partial\chi_B\partial\tilde{\eta}_B\rangle \\ &\qquad + h^2\langle \partial\chi_A\eta_A, \chi_B\partial(\tilde{\eta}_B - \eta_B)\rangle - h^2\langle \partial\chi_A\partial\eta_A, \chi_B(\tilde{\eta}_B - \eta_B)\rangle \\ &\qquad + t\langle \eta_A, \Delta V(\tilde{\eta}_B - \eta_B)\rangle - (\tilde{\mu}_B - \mu)\langle \chi_A\eta_A, \chi_B\tilde{\eta}_B\rangle.\end{aligned}$$

Recall that $\|\partial\chi_j\eta_j\| = \tilde{O}(e^{-\delta_0/h})$, $\|\partial\chi_j\tilde{\eta}_j\| = \tilde{O}(e^{-\delta_0/h})$, and $\|\tilde{\eta}_j - \eta_j\| = t\tilde{O}(e^{-\delta_j/h})$. We also have $(\tilde{P}_j(h) - \tilde{\mu}_j)(\tilde{\eta}_j - \eta_j) = -t\Delta V\eta_j + (\tilde{\mu}_j - \mu)\eta_j$. Then by proposition 5.7, we obtain

$$\begin{aligned}\|\partial(\tilde{\eta}_j - \eta_j)\|_{L^2(U)} &\leq \|\partial(\tilde{\eta}_j - \eta_j)\|_{H^2_h(U)} \\ &\leq C(\|(\tilde{P}_j(h) - \tilde{\mu}_j)(\tilde{\eta}_j - \eta_j)\|_{L^2(W)} + \|\tilde{\eta}_j - \eta_j\|_{L^2(W)}) \\ &\leq C(t\|\Delta V\eta_j\| + |\tilde{\mu}_j - \mu| + \|\tilde{\eta}_j - \eta_j\|) \\ &= t\tilde{O}(e^{-\delta_j/h}).\end{aligned}$$

Finally, $\|\tilde{\eta}_j - \eta_j\|_{L^2(\mathrm{Supp}(\Delta V))} = t\tilde{O}(e^{-2\delta_j/h})$. Then

$$\tilde{w}_{A,B} = w_{A,B} + t\langle \eta_A, \Delta V\eta_B\rangle + t\tilde{O}(e^{-(\delta_0 + \min(\delta_A,\delta_B))/h}).$$

□

7.3 Perturbed eigenvalues and eigenfunctions

We will now combine the previous results to determine $\tilde{E}_\pm$ and $\tilde{\Omega}_\pm$. The eigenvalues of an arbitrary symmetric 2×2-matrix

$$\begin{pmatrix} a & c \\ c & d \end{pmatrix}$$

solve $0 = (\lambda - a)(\lambda - d) - c^2 = \lambda^2 - (a+d)\lambda + ad - c^2$. Hence

$$\begin{aligned} \lambda_\pm &= \frac{1}{2}(a+d) \pm \frac{1}{2}\sqrt{(a+d)^2 - 4ad + 4c^2} \\ &= \frac{1}{2}(a+d) \pm \sqrt{\left(\frac{1}{2}(a-d)\right)^2 + c^2}. \end{aligned}$$

Let

$$y := \frac{1}{2}(a-d),$$

and let the eigenvectors in the basis $\{\tilde{e}_A, \tilde{e}_B\}$ be given by $(\lambda_1 \quad \lambda_2)^T \in \mathbb{R}^2$. Then we have

$$\begin{aligned} \begin{pmatrix} a\lambda_1 + c\lambda_2 \\ c\lambda_1 + d\lambda_2 \end{pmatrix} &= \begin{pmatrix} a & c \\ c & d \end{pmatrix}\begin{pmatrix} \lambda_1 \\ \lambda 2 \end{pmatrix} = \lambda_\pm \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} \\ &= \left(\frac{1}{2}(a+d) \pm \sqrt{\left(\frac{1}{2}(a-d)\right)^2 + c^2}\right)\begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}, \text{ hence} \\ c\begin{pmatrix} \lambda_2 \\ \lambda_1 \end{pmatrix} &= \begin{pmatrix} (-y \pm \sqrt{y^2 + c^2})\lambda_1 \\ (y \pm \sqrt{y^2+c^2})\lambda_2 \end{pmatrix}. \end{aligned}$$

So we obtain

$$\frac{\lambda_1}{\lambda_2} = \frac{y}{c} \pm \frac{1}{c}\sqrt{y^2 + c^2}. \tag{7.11}$$

Substituting:

$$\begin{aligned} a &= \tilde{\mu}_A + \tilde{O}(e^{-2\delta_0/h}) = \mu + t\tilde{O}(e^{-2\delta_A/h}) + \tilde{O}(e^{-2\delta_0/h}) \\ d &= \tilde{\mu}_B + \tilde{O}(e^{-2\delta_0/h}) = \mu + t\tilde{O}(e^{-2\delta_B/h}) + \tilde{O}(e^{-2\delta_0/h}) \\ y &= \frac{1}{2}(a-d) = t\tilde{O}(e^{-2\delta_A/h}) + t\tilde{O}(e^{-2\delta_B/h}) + \tilde{O}(e^{-2\delta_0/h}) \\ c &= \tilde{\beta} + \tilde{O}(e^{-2\delta_0/h}) = \beta + t\Re\langle \eta_A, \Delta V \eta_B \rangle + t\tilde{O}(e^{-(\delta_0 + \min(\delta_A, \delta_B))/h}) + \tilde{O}(e^{-2\delta_0/h}) \\ &= \tilde{O}(e^{-\delta_0/h}) \end{aligned}$$

Since the interaction term β is of order $\tilde{O}(e^{-\delta_0/h})$, we are interested in all terms of this order or lower. Without loss of generality, we can assume that $\delta_A \leq \delta_B$. Then we will consider the following two cases.

(a) $2\delta_A > \delta_0$, i.e. the perturbation is far away from both wells,

(b) $2\delta_A < \delta_0$, i.e. the perturbation is close to one of the wells.

We will treat each of these cases separately.

7.3.1 (a) $2\delta_A > \delta_0$

Setting $|t| = 1$, we obtain $y = \tilde{O}(e^{-2\delta_A/h}) + \tilde{O}(e^{-2\delta_0/h}) = \tilde{O}(e^{-2\min(\delta_0,\delta_A)/h})$. But then we have

$$y/c = \tilde{O}(e^{-(2\min(\delta_0,\delta_A) - \delta_0)/h})$$

where $2\min(\delta_0, \delta_A) - \delta_0 > 0$ due to $2\delta_A > 0$. Hence

$$
\begin{aligned}
\frac{\lambda_1}{\lambda_2} &= \frac{y}{c} \pm \frac{1}{c}\sqrt{y^2+c^2} = \frac{y}{c} \pm \sqrt{1+\left(\frac{y}{c}\right)^2} \\
&= \frac{y}{c} \pm \left(1 + \frac{1}{2}\left(\frac{y}{c}\right)^2 + \dots\right) \\
&= \pm 1 + \tilde{O}(e^{-(2\min(\delta_0,\delta_A)-\delta_0)/h}).
\end{aligned}
$$

So these eigenfunctions are split evenly over the two wells, i.e.

$$
\begin{aligned}
\tilde{\Omega}_\pm &= \frac{1}{\sqrt{2}}\tilde{e}_A \pm \operatorname{sign}(\beta)\frac{1}{\sqrt{2}}\tilde{e}_B + \tilde{O}(e^{-(2\min(\delta_0,\delta_A)-\delta_0)/h}) \\
&= \frac{1}{\sqrt{2}}\eta_A \pm \operatorname{sign}(\beta)\frac{1}{\sqrt{2}}\eta_B + \tilde{O}(e^{-(\delta_0,2\delta_A-\delta_0)/h}).
\end{aligned}
$$

So the perturbed eigenfunctions are the same as the unperturbed eigenfunctions, up to an exponentially small error.

7.3.2 (b) $2\delta_A < \delta_0$

Let $|t| > e^{-(\delta_0-2\delta_A)/h}$ as $h \to 0$. Then $y = t\tilde{O}(e^{-2\delta_A/h})$ and $c = \tilde{O}(e^{-\delta_0/h})$. Then

$$
\begin{aligned}
\sqrt{y^2+c^2} &= |y|\sqrt{1+\left(\frac{c}{y}\right)^2} = |y|\left(1+\frac{1}{2}\left(\frac{c}{y}\right)^2+\dots\right), \text{ hence} \\
\tilde{E}_\pm &= \mu + \frac{1}{2}t\langle\eta_A, \Delta V\eta_A\rangle \pm \frac{1}{2}|t|\langle\eta_A, \Delta V\eta_A\rangle + \frac{1}{t}\tilde{O}(e^{-(2\delta_0-2\delta_A)/h}), \text{ i.e.} \\
|\tilde{E}_+ - \tilde{E}_-| &= |t|\langle\eta_A, \Delta V\eta_A\rangle + \frac{1}{t}\tilde{O}(e^{-(2\delta_0-2\delta_A)/h}).
\end{aligned}
$$

Similarly, for the eigenfunction we can find that

$$
\begin{aligned}
\frac{\lambda_1}{\lambda_2} &= \frac{y}{c} \pm \frac{1}{c}\sqrt{y^2+c^2} = \frac{y}{c} \pm \frac{|y|}{c}\sqrt{1+\left(\frac{c}{y}\right)^2} \\
&= \frac{y}{c} \pm \frac{|y|}{c}\left(1+\frac{1}{2}\left(\frac{c}{y}\right)^2+\dots\right).
\end{aligned}
$$

In case $t > 0$, we find for $\tilde{\Omega}_+$ that $\lambda_1/\lambda_2 = 2y/c + \dots \to \infty$ as $h \to 0$, i.e. $\tilde{\Omega}_+ \approx \eta_A$, and for $\tilde{\Omega}_-$ that $\lambda_1/\lambda_2 = c/(2y) + \dots \to 0$ as $h \to 0$, i.e. $\tilde{\Omega}_- \approx \eta_B$. Similarly, if $t < 0$, we get $\tilde{\Omega}_+ \approx \eta_B$ and $\tilde{\Omega}_- \approx \eta_A$.

This means that an exponentially small perturbation can already 'tip over' the eigenfunctions $\Omega_\pm$ so they are localised in just one well! In case the perturbation raises the potential close to x_A, the lowest energy eigenfunction Ω_- is pushed away from x_A into the other well. If however the perturbation lowers the potential close to x_A, then the lowest energy eigenfunction Ω_- is pulled into x_A.

8 Outlook

We have looked at a one-dimensional symmetric double-well potential, and found that even an exponentially small perturbation could upset the balance enough to break the symmetry of the lowest energy eigenfunctions $\Omega_\pm$ to the maximum extend. It makes sense to ask if the same holds for eigenfunctions with higher energy than just the lowest two, or if we can obtain a similar result for a potential with more wells.

We obtained our result by explicitly calculating the eigenvalues and eigenfunctions of the relevant 2×2-matrices. In a more general setting, we would have to find the eigenvalues and eigenfunctions of an $M \times M$-matrix. Since there are known formulas that give the roots of an arbitrary cubic polynomial, our technique can potentially be generalised to a potential with three wells. However, this is no longer possible for $M > 3$. In that case, the error terms can potentially be simplified by using the WKB-approximation to approximate the single-well eigenfunctions $\eta_{j,k}$.

A Notation

Let X, Y be normed spaces, then the space of bounded linear operators $X \to Y$ is denoted $B(X, Y)$.

Definition A.1. *proposition 6.6 (multi-indices) An element $\alpha \in \mathbb{N}^n$ is called a multi-index.*

Let $n \in \mathbb{N}$ be the dimension, α a multi-index, $x \in \mathbb{R}^n$, $u : \mathbb{R}^n \to \mathbb{C}$ a map, $1 \leq j \leq n$, then we write:

- $\alpha = (\alpha_1, \ldots, \alpha_n)$
- $|\alpha| = \alpha_1 + \ldots + \alpha_n$
- $x^\alpha := x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n}$
- Note in particular that $(-1)^\alpha = (-1)^{|\alpha|}$
- $Du := \frac{1}{i} \nabla u = \frac{1}{i} \left(\frac{d}{dx_1} u, \ldots, \frac{d}{dx_n} u \right)$
- Sometimes we clarify in which variable we take the derivative by D_x or D_ξ.
- $D_j u := D_{x_j} u = \frac{1}{i} \frac{d}{dx_j} u$
- $D^\alpha u := \left(\frac{1}{i} \right)^{|\alpha|} \left(\frac{d^{\alpha_1}}{dx_1^{\alpha_1}} u \right) \ldots \left(\frac{d^{\alpha_n}}{dx_n^{\alpha_n}} \right)$
- $u, v : \mathbb{R}^n \to \mathbb{C}$, then $u \otimes v : \mathbb{R}^{2n} \to (\mathbb{C})$ is defined by $u \otimes v(x, y) := u(x)v(y)$.

Elements of $\mathbb{R}^{2n}$ are denoted $z = (x, \xi), w = (y, \eta)$ where $x, y, \xi, \eta \in \mathbb{R}^n$. The symplectic product on $\mathbb{R}^{2n}$ is denoted

$$\sigma(z, w) := \langle \xi, y \rangle - \langle x, \eta \rangle.$$

The Poisson bracket on $C^\infty(\mathbb{R}^{2n})$ is denoted

$$\{f, g\} = \langle \partial_\xi f, \partial_x g \rangle - \langle \partial_x f, \partial_\xi g \rangle.$$

B Basic inequalities

For reference, some basic inequalities will be collected here.

Lemma B.1. *(Inequalities involving real numbers) Let $a, b \in \mathbb{R}$, then*

$$ab \leq \frac{1}{2} \left(a^2 + b^2 \right), \tag{B.1}$$

$$a, b \geq 0 \implies a^2 + b^2 \leq (a + b)^2. \tag{B.2}$$

Lemma B.2. *(Inequalities involving $\langle x \rangle := (1 + |x|^2)^{1/2}$ where $x \in \mathbb{R}^n$)*

$$x < y \implies \langle x \rangle \leq \langle y \rangle, \tag{B.3}$$

$$\forall a > 0, \exists C_a > 0 \text{ such that } \langle x \rangle^2 \leq C_a(a + |x|^2), \tag{B.4}$$

$$\exists C > 0 \text{ such that } \forall M \in \mathbb{N}, M \geq n + 1, \text{ we have } \int_{\mathbb{R}^n} dx \left[\langle x \rangle^{-M} \right] \leq C. \tag{B.5}$$

Lemma B.3. *(Gradient estimate) Let $f : \mathbb{R}^n \to \mathbb{R}$ be C^2 and bounded from below. Write $f_\wedge := \inf f$ and assume that there is some constant $C > 0$ such that $|\partial_k \partial_l f| \leq C$ for all $1 \leq k, l \leq n$. Then there is a constant $C' > 0$ such that $|\partial_j f| \leq C'(f - f_\wedge)^{1/2}$ for all $1 \leq j \leq n$.*

C Functional analysis

Definition C.1. *(compact operators) Let X, Y be normed spaces. A linear operator $A : X \to Y$ is called compact if it satisfies the following two equivalent statements.*

(i) The image of the unit ball is precompact, i.e. $\overline{A(B(0,1))} \subset Y$ is compact.

(ii) For any bounded sequence $\{x_n\}_{n\in\mathbb{N}}$, the sequence $\{Ax_n\}_{n\in\mathbb{N}}$ containts a converging subsequence.

The set of compact operators $X \to Y$ will be denoted $K(X,Y)$. If $X = Y$, we will write $K(X)$ instead. It is easy to see that compact operators are bounded. The space $K(X,Y)$ inherits the topology from $B(X,Y)$.

Proposition C.2. *($K(X,Y)$ is a closed subspace) Let X be a normed space and let Y be a Banach space, then $K(X,Y)$ is a closed subspace of $B(X,Y)$.*

Definition C.3. *(Inverse operator) Let X, Y be normed spaces, then an operator $A \in B(X,Y)$ is called invertible if $\exists B \in B(Y,X)$ such that $BT = I_X$ and $TB = I_Y$. The operator B is called the inverse of A and is denoted $A^{-1} := B$.*

Lemma C.4. *Let X be a Banach space and let $A \in B(X)$ be an operator such that $\|A\| < 1$. Then the operator $I_X - A$ is invertible.*

Proof. Define for all $k \in \mathbb{N}$ the operator $B_k := \sum_{n=0}^{k} A^n$. This sequence converges due to $\|A\| < 1$. Then $\|(I_X - A)B_k - I_X\| = \|B_k(I_X - A) - I_X\| = \|-A^{k+1}\| \leq \|A\|^{k+1} \to 0$ as $k \to \infty$. So $I_X - A$ is indeed invertible with inverse $(I_X - A)^{-1} = \sum_{n\in\mathbb{N}} A^n$. □

Proposition C.5. *(Approximate inverse gives rise to an inverse) Let X, Y be Banach spaces and let $A \in B(X,Y)$. If there are $B_1, B_2 : Y \to X$ and $R_1 \in B(Y)$ and $R_2 \in B(X)$ such that $AB_1 = I_Y + R_1$, $B_2A = I_X + R_2$, and $\|R_1\| < 1$, $\|R_2\| < 1$, then A is invertible.*

Proof. Per the previous lemma, $I_Y + R_1$ and $I_X + R_2$ are invertible with inverses $(I_Y + R_1)^{-1} = \sum_{n\in\mathbb{N}}(-R_1)^n$ and $(I_X + R_2)^{-1} = \sum_{n\in\mathbb{N}}(-R_2)^n$. Define the operators $C_1 := B_1(I_Y + R_1)^{-1}$ and $C_2 := (I_X + R_2)^{-1}B_1$. Then $AC_1 = I_Y$ and $C_2A = I_X$. For all $y \in Y$ we obtain $C_1y = C_2AC_1y = C_2y$, hence $A^{-1} = C_1 = C_2$, □

Definition C.6. *(Spectrum of an operator) Let H be a Hilbert space and let $A : H \to H$ be a bounded linear operator, then its spectrum is $\sigma(A) := \{\lambda \in \mathbb{C} \mid A - \lambda I$ is not invertible$\}$.*

Proposition C.7. *Let H be a Hilbert space, $A : H \to H$ a bounded linear operator, then the spectrum $\sigma(A)$ is compact.*

Definition C.8. *(Adjoint) Let H_1, H_2 be Hilbert spaces and let $A : H_1 \to H_2$ be a bounded linear operator. Then its adjoint A^* is the unique bounded linear operator $A^* : H_2 \to H_1$ such that $\langle v, Au\rangle_{H_2} = \langle A^*v, u\rangle_{H_1}$ for all $u \in H_1, v \in H_2$. An operator $A : H \to H$ is called self-adjoint if $A = A^*$.*

Proposition C.9. *Let H be a Hilbert space and let $A : H \to H$ be a self-adjoint bounded linear operator, then $\sigma(A) \subset \mathbb{R}$. Moreover, if $A_\wedge := \inf \sigma(A)$ and $A_\vee := \sup \sigma(A)$, then $A_\wedge\|u\|^2 \leq \langle u, Au\rangle \leq A_\vee\|u\|^2$ for all $u \in H$.*

References

[1] Lawrence Evans, *Partial differential equations second edition*, AMS, 2010.

[2] Bernard Helffer, *Semi-classical analysis for the Schrödinger operator and applications*, Springer-Verlag, Lecture notes in mathematics 1336, 1987.

[3] Bernard Helffer, Johannes Sjöstrand, *Multiple wells in the semi-classical limit I*, Comm. in partial differential equations, 1984.

[4] Bernard Helffer, Johannes Sjöstrand, *Puits multiples en limite semi-classique. II. Interaction moléculaire. Symétries. Perturbation*, Annales de l'I. H. P., 1985.

[5] Jean-Michel Bony, Gerd Grubb, Lars Hörmander, Hikosaburo Komatsu, Johannes Sjöstrand, *Microlocal analysis and applications*, Springer-Verlag, 1989.

[6] Walter Rudin, *Functional analysis*, McGraw-Hill, Inc, 1991.

[7] Barry Simon, *Semiclassical analysis of low lying eigenvalues IV. The flea on the elephant*, California institute of technology, 1984.

[8] Maciej Zwroski, *Semiclassical analysis*, AMS, 2012.

[9] G. Jona-Lasinio, F. Martinelli, E. Scoppola, *New approach to the semiclassical limit of quantum mechanics. I. Multiple tunnelings in one dimension*, Comm. Math. Phys. 80, no. 2, 223-254 1981.

[10] S. Graffi et al., *Tunneling instability via perturbation theory*, J. Phys. A: Math. Gen. 17 2935, 1984.