Two-term Szegő theorem for generalised anti-Wick operators

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Declaration

I, James Oldfield, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

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Abstract

This thesis concerns operators whose Weyl pseudodifferential operator symbol is the convolution of a function that is smooth and of fixed scale with a function that is discontinuous and dilated by a large asymptotic parameter. A special case of these operators of particular interest is the class of generalised anti-Wick operators, and then the fixed-scale part corresponds to the window functions while the dilated part is the generalised anti-Wick symbol.

The main result is a Szegő theorem that gives two terms in the asymptotic expansion of the trace of a function of the operator. Two variants are proved: in one the discontinuity must occur on a C^2 surface but the symbol may have unbounded support, while in the other the set on which the discontinuity occurs may be much more general (most importantly, it must be Lipschitz and piecewise C^2), but the symbol must be compactly supported. A corollary of this theorem is two terms in the asymptotic expansion of the eigenvalue counting function when the smooth part of the symbol is constant. Prior to this work, only one term in each of these expansions was known. It is also shown that the remainder in the Szegő theorem is larger for a class of examples where the boundary has a cusp; this shows that the Lipschitz condition in the main theorem cannot be removed without weakening the conclusion.

A significant step in the proof of this Szegő theorem is a composition result for Weyl pseudodifferential operators that may be of more general interest: the symbol of the composition is expressed as a finite series in the standard form, but with an explicit trace norm and operator norm bound of the remainder expressed using the symbols in a similar way to the first excluded term. In the one-term case, this is used to derive an analogous trace norm bound for approximating the Weyl symbol of a function of an operator. Another important part of the proof of the Szegő theorem is the use of standard tubular neighbourhood theory to describe the geometry of the surface on which the discontinuity occurs; this is derived in full for the necessary conditions.

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Contents

Notation

Where a notation is mentioned in the introduction chapter but not defined in full until a later chapter, the page number refers to its later definition.

$\lesssim \cdots$	Bounded above by a constant multiple (alternative notation for $O(\cdots)$)	99
$\nabla \otimes a$	Jacobian matrix $(\nabla a^{\mathrm{T}})^{\mathrm{T}}$	70
$\lVert A \rVert_1$	Trace norm of the operator A	29
A_0, A_1	Asymptotic terms in Szegő theorem for generalised anti-Wick operators	101
$\mathscr{A}_{\varphi_2,\varphi_1}[a]$	Generalised anti-Wick operator with windows φ_1, φ_2	22
$\mathscr{A}_{\varphi}[a]$	Generalised anti-Wick operator with the same function for φ_1 and φ_2	23
$B_t(\boldsymbol{z})$	Open ball of radius t about the point $\boldsymbol{z} \in \mathbb{R}^m$	72
$B_t(\mathit{\Gamma})$	Set of points within distance t of the set $\mathit{\Gamma} \subseteq \mathbb{R}^m$	72
$C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$	Space of bounded smooth functions with bounded derivatives on $\mathbb{R}^{2d}$	28
$\chi_{\mathit{\Omega}}$	Indicator function of the set $\mathit{\Omega}$	14
e	Exponential map on a manifold $\mathit{\Gamma}$	72
$\mathrm{ext}_t(\mathit{\Gamma})$	Extension of extensible set $\mathit{\Gamma}$ by radius t	84
F_j	Term in asymptotic expansion of $\mathrm{op}[p]\,\mathrm{op}[q]$	35
$\mathscr{F}_{\varphi}$	Short-time Fourier transform with window φ	22
$\mathit{\Gamma}^{(\mathrm{i})}$	Set contained within a strongly extensible manifold	83
$\mathit{\Gamma}^{(\mathrm{o})}$	Set containing an extensible manifold	83
$\mathit{\Gamma}_i$	In Condition 5.2.7, the C^2 extensible pieces making up $\partial \mathit{\Omega}$	102
$\mathsf{M}^{G,D}(F)$	Weighted Sobolev norm of F with D derivatives in L^1	64
μ_k	k-dimensional Hausdorff measure	18
$\mu_k(\mathrm{d}\boldsymbol{x})$	k-dimensional volume element (as in $\int_{\partial\mathit{\Omega}} f(\boldsymbol{x})\mu_{m-1}(\mathrm{d}\boldsymbol{x})$ when $\mathit{\Omega} \subseteq \mathbb{R}^m$)	18
$N(A, I)$	Number of eigenvalues of the operator A in the set I	103
$\mathsf{N}_p^D(a)$	Sobolev norm of a with D derivatives in L^p	64
$N_t^{\boldsymbol{u}}$	Normal space at $\boldsymbol{u}$ (points of size less than t if subscript included)	70
N_t	Normal bundle (points of size less than t if subscript included)	72
$\boldsymbol{n}(\boldsymbol{u})$	(For $\boldsymbol{u} \in \partial\mathit{\Omega}$) Inward normal vector at $\boldsymbol{u}$ on the boundary of a domain $\mathit{\Omega}$	79
$\boldsymbol{n}(\boldsymbol{z})$	(For $\boldsymbol{z} \in \mathrm{tub}(\partial\mathit{\Omega})$) Extension of normal vector field from $\partial\mathit{\Omega}$ to $\mathrm{tub}(\partial\mathit{\Omega})$	79

Chapter 1

Introduction

In the broadest sense, Szegő theorems could be described as asymptotic spectral results about operators that include some sort of scaled projection and some sort of multiplication in Fourier space. The Szegő theorem proved in this thesis is for a class of operators that includes generalised anti-Wick operators, which will be described later in this chapter, where multiplication in Fourier space is achieved with the short-time Fourier transform and something like a projection is achieved by multiplying by an indicator function (or other discontinuous function).

The interest in this theorem is strongly related to the Szegő theorem for pseudodifferential operators with discontinuous symbol. This, in turn, can be traced back in two directions.

The first way has its roots in the original Szegő theorems for Toeplitz matrices. Here the asymptotic parameter is the size of the matrix, and the multiplication in Fourier space is multiplication by a function whose Fourier coefficients match the matrix entries. The original Szegő theorem, proved by Szegő (1915), gives the limit of $\sqrt[n]{\det T_n}$ as $n \to \infty$. This result and some of its generalisations are described in §1.1. The continuous analogues are called truncated Wiener–Hopf operators, where the action on sequences is replaced by action on functions of $\mathbb{R}^d$, and summation of Fourier series is replaced by the Fourier transform. These operators and the corresponding results are described in §1.2, culminating in a Szegő theorem by Widom (1982) and Sobolev (2013) for truncated Wiener–Hopf operators that have discontinuous symbols and may include a multiplicative factor.

The other direction this theorem can be traced from is semiclassical analysis. The most common interpretation of this is that it concerns the extent to which classical mechanics approximates quantum mechanics on macroscopic scales. An important result in this area is the functional calculus for semiclassical pseudodifferential operators. In §1.3 the result by Widom (1982) and Sobolev (2013) is put into this context as a weak version of this functional calculus in the case that the symbol is discontinuous in both variables. Now the asymptotic parameter corresponds to the semiclassical parameter h, instead of being the analogue of the size of the matrix.

A more tractable alternative to pseudodifferential operators are generalised anti-Wick operators, also known as short-time Fourier transform multipliers. The short-time Fourier transform is both widely studied and widely used in practice, but until the result in this thesis was found, only a weak Szegő theorem was known for the corresponding operators. These operators and the relevant results, including the new one, are discussed in §1.4.

In fact the result proved in this thesis applies to a more general class of operators than generalised anti-Wick operators: that of operators whose Weyl pseudodifferential operator symbol is the convolution of a function that is smooth and of fixed scale with a function that is discontinuous and dilated by a large asymptotic parameter. This class of operators is discussed in §1.5, which includes a description of the two main steps of the proof of the Szegő theorem and an outline of the remaining chapters.

1.1 Toeplitz matrices

A *Toeplitz matrix* is a matrix of the form $(b_{i-j})_{i,j=0}^{n}$; that is, it is constant along the diagonals. For example, when $n=3$ the general form of a Toeplitz matrix is

$$\begin{pmatrix} b_0 & b_{-1} & b_{-2} & b_{-3} \\ b_1 & b_0 & b_{-1} & b_{-2} \\ b_2 & b_1 & b_0 & b_{-1} \\ b_3 & b_2 & b_1 & b_0 \end{pmatrix}.$$

The semi-infinite matrix defined the same way, with entries $(b_{i-j})_{i,j=0}^{\infty}$, is called a *Toeplitz operator*. The effect of multiplying a Toeplitz matrix by a vector $\boldsymbol{x}\in\mathbb{C}^{n+1}$ is thus

$$(T\boldsymbol{x})_i=\sum_{j=0}^{n} b_{i-j}x_j.$$

This is the discrete analogue of convolution with the indices truncated to the range $0,\dots,n$. Just as the usual convolution can be expressed in terms of multiplication and the Fourier transform, the action of multiplication by a Toeplitz matrix can be expressed in terms of multiplication and Fourier series. To do this, let us define some notation: Let $\mathscr{F}_{\mathrm{s}}\colon \ell^2(\mathbb{Z})\to L^2([0,2\pi])$ be the unitary operator that takes a doubly-infinite sequence to the function of $[0,2\pi]$ with those Fourier coefficients, i.e.

$$(\mathscr{F}_{\mathrm{s}}\, b)(x)=\frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} b_n\,\mathrm{e}^{\mathrm{i}nx}, \qquad (\mathscr{F}_{\mathrm{s}}^{-1}a)_n=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} a(x)\mathrm{e}^{-\mathrm{i}nx}\,\mathrm{d}x.$$

Let χ_{Ω} be the indicator function of Ω, which equals 1 for points in Ω and equals 0 for points in the complement Ω^{c}. When a function appears in a composition of operators it acts as an operator by multiplication. Then multiplication by a Toeplitz matrix is

$$T_n[a]:=\chi_{\{0,\dots,n\}}\mathscr{F}_{\mathrm{s}}^{-1}a\mathscr{F}_{\mathrm{s}}\chi_{\{0,\dots,n\}}, \text{ where } a:=\sqrt{2\pi}\mathscr{F}_{\mathrm{s}}b.$$

As reflected in the notation $T_n[a]$, we usually identify Toeplitz matrices by the function a, called the *symbol* of the matrix, rather than the sequence b.

The asymptotic properties of Toeplitz matrices as $n \to \infty$ are of particular interest. To express these we will use two standard asymptotic notations, defined as n approaches some limit by

$$
\begin{aligned}
f(n) = g(n) + o(r(n)) \quad &\iff \quad \frac{f(n) - g(n)}{r(n)} \to 0, \\
f(n) = g(n) + O(r(n)) \quad &\iff \quad \left| \frac{f(n) - g(n)}{r(n)} \right| \leqslant C,
\end{aligned}
$$

with the second equation holding for some number $C \geqslant 0$ for all n close enough to the limit (or all sufficiently large n if the limit is $+\infty$).

In general it is difficult to find information about the individual eigenvalues of $T_n[a]$, so there has been much study of broader information about eigenvalues. A landmark early theorem of this type was proved by Szegő (1915) (see also the book by Grenander and Szegő, 1958, 5.2 (c)(ii)) that had earlier been conjectured by Pólya (1914). The original statement of the theorem required that the symbol be continuous and strictly positive. (Here and elsewhere in this section, regularity requirements on the symbol assume that 0 and 2π are identified; in this case, continuity requires that $a(0) = a(2\pi)$.) Then we have

$$
\lim_{n\to\infty} \sqrt[n]{\det T_n[a]} = \exp\left(\frac{1}{2\pi} \int_0^{2\pi} \log a(\omega)\, \mathrm{d}\omega \right).
$$

Taking the logarithm of this expression and using the fact that $\det T_n[a]$ is the product of the eigenvalues of $T_n[a]$ whereas $\operatorname{tr}\log T_n[a]$ is the sum of their logarithms, we can express this relationship as $n \to \infty$ by

$$
\operatorname{tr}\log T_n[a] = \frac{n}{2\pi} \int_0^{2\pi} \log a(\omega)\, \mathrm{d}\omega + o(n).
$$

Since the original result was published, the Szegő theorem has been subject to intensive study to a degree that one could not hope to be fully covered here. Instead, for more information the reader is referred to the introductory book by Böttcher and Silbermann (1998, Chapter 5) and their more detailed monograph (Böttcher and Silbermann, 2006, Chapter 10), and also to the book by Simon (2011) for the connection with orthogonal polynomials. However, there are some particular developments of the theorem that will be important here, which are discussed below with references to the earliest results along those lines.

- **Stronger asymptotic result:** One direction in which the Szegő theorem can be strengthened is by including more asymptotic information in the conclusion. In fact Szegő proved his original theorem by showing that

$$
\operatorname{tr}\log T_n[a] - \operatorname{tr}\log T_{n-1}[a] = \frac{1}{2\pi} \int_0^{2\pi} \log a(\omega)\, \mathrm{d}\omega + o(1).
$$

  which is a stronger statement and came to be known as the *(first) Szegő theorem*. A result with a stronger still conclusion was later proved by Szegő (1952) (see also Grenander and Szegő, 1958, §5.5). This says that when the symbol a is sufficiently regular (twice differentiable will suffice) and strictly positive we have

$$\operatorname{tr}\log T_n[a] = \frac{n}{2\pi}\int_0^{2\pi} \log a(\omega)\,\mathrm{d}\omega + O(1).$$

In fact he also found the constant term with $o(1)$ remainder, which can be written explicitly in terms of the Fourier coefficients of $\log a$, but its exact form will not be relevant here. This is known as the *strong Szegő theorem*.

- **More general function of the matrix:** Another variation on the Szegő theorem is to replace log with a more general function of the operator. This was proved by Szegő (1917) (and in the more widely distributed article, also by Szegő, 1920, Satz XVIII). He showed that when a is locally integrable and real valued and f is a continuous function defined on an interval containing the image of a, we have

  $$\operatorname{tr} f\big(T_n[a]\big) = \frac{n}{2\pi}\int_0^{2\pi} f\big(a(\omega)\big)\,\mathrm{d}\omega + o(n).$$

  Clearly the original theorem can be recovered from this by setting $f(t) = \log t$ for $t > 0$. In fact Szegő showed the other direction: this formula can be recovered for arbitrary continuous f by applying the original theorem with varying choices of symbol. A particular use of the version with general f is that it implies the result for the indicator function $f = \chi_I$, even though it is discontinuous, when $I \subseteq \mathbb{R}$ is a region for which $a^{-1}(\partial I)$ has zero measure (see for example Böttcher and Silbermann, 1998, §5.5). Let μ_1 denote the one dimensional Lebesgue measure. Then this result says that number of eigenvalues of $T_n[a]$ in I as $n \to \infty$ satisfies

  $$N\big(T_n[a], I\big) = \frac{n}{2\pi}\mu_1(a^{-1}(I)) + o(n).$$

- **Weaker regularity requirements on the symbol:** It was realised by Pólya that, in the original Szegő theorem, the requirement that the symbol be continuous can be weakened to it simply being locally integrable (see Szegő, 1915, footnote on p. 503). For the strong theorem, Fisher and Hartwig (1969, §IV) made a quite general conjecture that included discontinuous symbols (and also singular symbols and symbols for which $\inf a = 0$). The first general result for discontinuous symbols was proved by Widom (1973, §XIII). To relate formulae of this type to those of the next section, we may choose discontinuous symbol $1+\chi_\Lambda a$, where Λ is a subinterval of $[0, 2\pi]$ and a is a sufficiently smooth real valued function with $\min a > -1$; we then have

  $$\operatorname{tr}\log(I_n + T_n[\chi_\Lambda a]) = \frac{n}{2\pi}\int_\Lambda \log(1+a(\omega))\,\mathrm{d}\omega + \frac{\log n}{(2\pi)^2}\sum_{\omega\in\partial\Lambda}\big(\log(1+a(\omega))\big)^2 + O(1).$$

- **Higher dimensions:** We can obtain a higher-dimensional analogue by replacing the one dimensional Fourier series operator with the higher dimensional analogue $\mathscr{F}_\mathrm{s}\colon \ell^2(\mathbb{Z}^d) \to L^2([0,2\pi]^d)$; i.e.

$$(\mathscr{F}_\mathrm{s}\, b)(\boldsymbol{x}) = \frac{1}{(2\pi)^{d/2}} \sum_{\boldsymbol{n}\in\mathbb{Z}^d} b_{\boldsymbol{n}}\, \mathrm{e}^{\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}, \qquad (\mathscr{F}_\mathrm{s}^{-1} a)_{\boldsymbol{n}} = \frac{1}{(2\pi)^{d/2}} \int_{[0,2\pi]^d} a(\boldsymbol{x})\mathrm{e}^{-\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x}.$$

  For $a \in L^\infty([0,2\pi]^d)$ and $\Omega \subseteq \mathbb{R}^d$ we now define $T_n[a;\Omega] := \chi_{n\Omega}\mathscr{F}_\mathrm{s}^{-1} a \mathscr{F}_\mathrm{s}\chi_{n\Omega}$. (In one dimension the operator is retrieved by putting $\Omega = [0,1]$.) Linnik (1975) showed that when a is real-valued and sufficiently regular and Ω has sufficiently smooth boundary, we have

$$\operatorname{tr}\log T_n[a;\Omega] = \frac{C(n,\Omega)}{(2\pi)^d} \int_{[0,2\pi]^d} \log a(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega} + O(n^{d-1})$$

  as $n \to \infty$, where $C(n,\Omega)$ is the number of points in $n\Omega \cap \mathbb{Z}^d$. Linnik also found the coefficient of n^{d-1} with $o(n^{d-1})$ error.

- **Non self-adjoint operators:** The above results all assume that a is real-valued, which implies that the matrix $T_n[a]$ is self-adjoint (and conversely if $T_n[a]$ is self-adjoint then a is real almost everywhere). Proving Szegő theorems for complex-valued symbols is significantly more difficult, particularly because density arguments used in the self-adjoint case no longer apply. Indeed, Schmidt and Spitzer (1960) pointed out that Kac (1954) had generalised the strong Szegő theorem to a class of complex-valued symbols in the course of proving another result, but only for polynomial functions of the operator. Investigations into the theorem with the logarithm of the operator were started by Reich (1962) and Devinatz (1966), who proved the weak Szegő theorem for complex-valued symbols under various, rather restrictive, conditions on the symbol.

1.2 Truncated Wiener–Hopf operators

In this section we discuss *truncated Wiener–Hopf operators*, which are the continuous analogue of Toeplitz matrices. Multiplication by a Toeplitz matrix is discrete convolution with a sequence with indices truncated to the range $0,\dots,n$, whereas the action of a truncated Wiener–Hopf operator is conventional convolution with a function of $\mathbb{R}$ truncated to the range $[0,\alpha]$. We now write this out explicitly in the multidimensional case. Let b be a function on $\mathbb{R}^d$ and let $\Omega \subseteq \mathbb{R}^d$; then for $f \in L^2(\mathbb{R}^d)$ and $\boldsymbol{x} \in \alpha\Omega$, we set

$$Tf(\boldsymbol{x}) := \int_{\alpha\Omega} b(\boldsymbol{x}-\boldsymbol{y})f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

As with Toeplitz matrices, this may fruitfully be written in terms of multiplication and the Fourier transform. We use the convention for the Fourier transform that

$$\mathscr{F}f(\xi) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y};$$

in particular, $\mathscr{F}: L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is a unitary operator. Then the truncated Wiener–Hopf operator is given by

$$T_\alpha[a;\Omega] := \chi_{\alpha\Omega}\mathscr{F}^{-1}a\mathscr{F}\chi_{\alpha\Omega}, \text{ where } a := (2\pi)^{d/2}\mathscr{F}b.$$

A Szegő theorem for truncated Wiener–Hopf operators was found by Kac (1954) with more information found by Akhiezer (1964). This says that for $\Omega := [0,1]$ and a a sufficiently regular non-negative function on $\mathbb{R}$, as $\alpha \to \infty$ we have

$$\operatorname{tr}\log(I + T_\alpha[a;\Omega]) = \frac{\alpha}{2\pi}\int_{-\infty}^{\infty} \log(1 + a(\xi))\,\mathrm{d}\xi + O(1).$$

This matches the formula for Toeplitz matrices when we apply the function $\log(1+t)$ to the operator. Although not explicitly written here, the constant term was also found with remainder $o(1)$, and the expression for that is also analogous to the discrete case.

As with the Szegő theorem for Toeplitz matrices, there are many ways to extend the Szegő theorem for truncated Wiener–Hopf operators:

- **Higher dimensions:** The higher dimensional result was found by Widom (1960) up to the second term (of order α^{d-1}). It says that, for sufficiently regular real-valued a and a simple enough set $\Omega \subseteq \mathbb{R}^d$, we have

  $$\operatorname{tr}\log(I + T_\alpha[a;\Omega]) = \frac{\alpha^d}{(2\pi)^d}\mu_d(\Omega)\int_{\mathbb{R}^d} \log(1 + a(\boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi} + O(\alpha^{d-1}),$$

  where μ_k is the k-dimensional Hausdorff measure, so $\mu_d(\Omega)$ is the volume of the region Ω. Again, this formula is analogous to the discrete case.

- **Multiplicative factors:** Let us use the notation, for any sufficiently smooth and quickly-decaying a, that for each $u \in L^2(\mathbb{R}^d)$ we set

  $$\operatorname{op}_1^{\mathrm{a}}[a]u(\boldsymbol{x}) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{\xi}} a(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi})u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\xi}.$$

  If a depends only on $\boldsymbol{x}$ or $\boldsymbol{y}$ then $\operatorname{op}_1^{\mathrm{a}}[a]$ is the operator that just multiplies by this function. If a depends only on $\boldsymbol{\xi}$ then by the Fourier inversion theorem it is a convolution operator; in particular, Wiener–Hopf operators can be written as $T_\alpha[a;\Omega] = \chi_{\alpha\Omega}\operatorname{op}_1^{\mathrm{a}}[a(\boldsymbol{\xi})]\chi_{\alpha\Omega}$. Widom (1974, §6) proved a Szegő theorem for operators of this form (including the multiplications by $\chi_{\alpha\Omega}$) but with a allowed to depend on $\boldsymbol{x}$ and $\boldsymbol{y}$ (in a restricted way) as well as $\boldsymbol{\xi}$, which he called "variable convolution operators". In this case the Szegő theorem becomes

  $$\operatorname{tr}\log(I + T_\alpha[a;\Omega]) = \frac{\alpha^d}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\Omega} \log(1 + a(\boldsymbol{x},\boldsymbol{x},\boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{\xi} + O(\alpha^{d-1}).$$

- **More general function of the operator:** Widom (1980) observed that for general f the formula should be

  $$\operatorname{tr} f(T_\alpha[a;\Omega]) = \frac{\alpha^d}{(2\pi)^d}\mu_d(\Omega)\int_{\mathbb{R}^d} f(a(\boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi} + O(\alpha^{d-1}),$$

and also found the α^{d-1} term with $o(\alpha^{d-1})$ error. However, it was only proved for analytic functions of the operator (albeit under very general conditions for the symbol). He allowed more general f in the results discussed in the next two bullet points (Widom, 1982, 1985).

- **Stronger asymptotic result:** The initial result by Kac included two terms (the α and constant term), so unlike the discrete case this much was known from the outset. However, even higher order terms in the expansion have been found. Roccaforte (1984) found the third term in arbitrary dimension (of order α^{d-2}) when $f(t) = \log(1+t)$, and also for more general functions of the operator but with the condition that these functions be analytic. A complete asymptotic expansion was found by Widom (1985), also in arbitrary dimension but this time with general functions of the operator that need not be analytic, and also allowing the operator to include a multiplicative dependence as described above. The geometric meaning of these terms was later clarified by Roccaforte (2013) using geometric theory similar to some that will be important in this thesis (see Chapter 4).

- **Weaker regularity requirements on the symbol:** The results most relevant to this thesis are where the symbol is discontinuous. The relevant results also allow the symbol to depend on $\boldsymbol{x}$ and $\boldsymbol{y}$ in the way described above, but with the symmetry restriction $a(\boldsymbol{x},\boldsymbol{y},\xi) = \frac{1}{2}\big(p(\boldsymbol{x},\xi) + \overline{p(\boldsymbol{y},\xi)}\big)\chi_\Lambda(\xi)$, which ensures that the operator is self-adjoint. An early result of this type was proved by Landau and Widom (1980), and it was proved for more general symbols with general function of the operator by Widom (1982). Both of these were only for one dimension, and a later attempt by Widom (1990) to prove the result in higher dimensions only resulted in a theorem with the very restrictive condition that Ω or Λ are a half-space (and in particular, we cannot choose $p \equiv 1$, because that would not result in a trace class operator). The full higher dimensional result was ultimately proved by Sobolev (2013, following a 2009 preprint) when the boundaries of Ω and Λ are sufficiently smooth (for operators which, by Lemma 4.5 of that work, may be put in the form discussed here). The conclusion of the result is that

  $$\operatorname{tr} f(T_\alpha[a;\Omega]) = \alpha^d A_0 + \alpha^{d-1}\log\alpha\, B + o(\alpha^{d-1}\log\alpha)$$

  as $\alpha \to \infty$. In a similar way to other results, the first term A_0 is the integral over $\Omega\times\Lambda$ of f applied to $\frac{1}{2}\big(p(\boldsymbol{x},\xi) + \overline{p(\boldsymbol{x},\xi)}\big)$. However, there is now an additional term of order $\alpha^{d-1}\log\alpha$, with a coefficient B which may be written explicitly as an integral over $\partial\Omega\times\partial\Lambda$. This result will be revisited in §1.3 from a slightly different perspective.

  Sobolev (2015) later relaxed the condition on the regularity of the boundary of Ω and Λ, instead simply requiring that they be Lipschitz and piecewise smooth, with the same formula holding. A particularly interesting feature of this is that the prior results may have given the mistaken impression that the $\alpha^{d-1}\log\alpha$ term depends on the "corners" of the discontinuity, because in one dimension $\Omega\times\Lambda$ is a rectangle and $\partial\Omega\times\partial\Lambda$ is the set of its vertices. However, even when there are other non-smooth points in $\partial(\Omega\times\Lambda)$, it remains true that the logarithmic term depends only on the product of the individual boundaries $\partial\Omega\times\partial\Lambda$.

As with the Toeplitz matrix result, one benefit of having a result with general f is that, when $p\equiv 1$, by an approximation argument we can substitute $f=\chi_{[\delta,\infty)}$ to obtain an eigenvalue counting result. It gives us an explicit formula (Sobolev, 2013, Remark 2.8) with the same asymptotic form as the Szegő theorem, so now A_0 is the volume of $\Omega\times\Lambda$ and (counting eigenvalues greater than $\delta\in(0,1)$) the second term is

$$B=\frac{1}{(2\pi)^{d+1}}\mu_{d-1}(\partial\Omega)\mu_{d-1}(\partial\Lambda)\log\left(\frac{1-\delta}{\delta}\right).$$

- **Non self-adjoint operators:** As with Toeplitz operators, it is significantly harder to prove a Szegő theorem for truncated Wiener–Hopf operators when we drop the requirement that the operator be self-adjoint. In the case of most interest here, the theorem by Sobolev when a has a discontinuity in ξ, there is a non self-adjoint analogue with $a(\boldsymbol{x},\boldsymbol{y},\xi)=p(\boldsymbol{x},\xi)\chi_\Lambda(\xi)$ or $a(\boldsymbol{x},\boldsymbol{y},\xi)=p(\boldsymbol{y},\xi)\chi_\Lambda(\xi)$, but then f is restricted to analytic functions.

1.3 Semiclassical pseudodifferential operators

In this section we will consider the final Szegő theorem discussed in the previous section, which is for truncated Wiener–Hopf operators with discontinuous symbol, but with a slightly different interpretation: instead of thinking of the asymptotic parameter as an analogue of the size of a Toeplitz matrix, we will think of it as a semiclassical parameter.

Pseudodifferential operators have applications in many different fields, including analysis of partial differential equations (for which they were first developed) and time–frequency analysis. There is a vast literature on the subject, but a good starting point is the excellent texts by Folland (1989) and Martinez (2001). The area of most interest here is in quantum mechanics, which we will now look at very briefly.

In our universe, quantum mechanical effects are most noticeable at extremely small length scales. For a given particle, the relevant scale is its Compton wavelength, which is proportional to Planck's constant h. The *Bohr correspondence principle* states that quantum mechanics is approximated by classical mechanics on macroscopic scales. A form of this can be stated more precisely as follows.

In classical mechanics, physical quantities are known as *observables* and are functions of generalised coordinates; for example, a particle with momentum and position $(p,q)\in\mathbb{R}^{3+3}$ has kinetic energy $\frac{1}{2}|p|^2/m$. In quantum mechanics, observables are now self-adjoint operators; for example, a particle could be described by a wave function $\psi\in L^2(\mathbb{R}^3)$ and the kinetic energy observable is then given by $-\frac{1}{2}\hbar^2\Delta/m$, where Δ is the Laplacian and $\hbar=h/2\pi$. A mapping $a\mapsto\operatorname{op}_h[a]$ from classical observables to their corresponding quantum mechanical observables is called a *quantisation*. The Bohr correspondence principle now states that, in some sense, $\mathrm{op}_h[a]$ is like the classical observable a when h is asymptotically small. In particular, we have the approximate relationships

$$\mathrm{op}_h[a]\,\mathrm{op}_h[b] \approx \mathrm{op}_h[ab], \qquad f(\mathrm{op}_h[a]) \approx \mathrm{op}_h[f(a)].$$

In both cases, the operator on each side of the equation acts on the scale of the large quantity $1/h$ in some sense, and we would expect the error to be at least as small as constant scale.

The standard semiclassical quantisations are given by pseudodifferential operators defined for $\tau \in [0,1]$ by

$$(\mathrm{op}_h^\tau[q]u)(\boldsymbol{x}) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi} q(\tau\boldsymbol{x} + (1-\tau)\boldsymbol{y}, h\xi) u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\xi.$$

When $q(\boldsymbol{x},\xi)$ is a function only of $\boldsymbol{x}$ these all simply describe a multiplication operator. When q is a power of ξ with a multi index $\boldsymbol{k} \in \mathbb{N}_0^d$ these all satisfy $\mathrm{op}_h^\tau[\mathrm{i}^{|\boldsymbol{k}|}\xi^{\boldsymbol{k}}] = h^{|\boldsymbol{k}|}\partial^{\boldsymbol{k}}$, so pseudodifferential operators are a generalisation of differential operators. In particular, they are consistent with the kinetic energy example: for all $\tau \in [0,1]$ we have $\mathrm{op}_\hbar^\tau\big[\frac{1}{2}|\xi|^2/m\big] = -\frac{1}{2}\hbar^2\Delta/m$. Particularly common quantisations include the *left* (or *Kohn–Nirenberg*) *quantisation* given by $\tau = 1$, which we will denote $\mathrm{op}_h^1[q]$, and the *Weyl quantisation* given by $\tau = \frac{1}{2}$, which has many particularly useful properties, and which we will denote $\mathrm{op}_h^{\mathrm{W}}[q]$.

A semiclassical functional calculus for Weyl pseudodifferential operators with smooth symbols was developed by Helffer and Robert in the early 1980's (see the book by Robert, 1987, for individual citations, and Théorème (III-11) for the result). A simplified statement of this is that, for any sufficiently smooth symbol a and any $n \in \mathbb{N}_0$, we have

$$f\big(\mathrm{op}_h^{\mathrm{W}}[a]\big) \approx \frac{1}{(2\pi h)^d} \sum_{j=0}^{n} h^j\,\mathrm{op}_h^{\mathrm{W}}[a_j],$$

where a_j can be written in terms of a and f, and in particular $a_0(\boldsymbol{z}) = f(a(\boldsymbol{z}))$ and $a_1 \equiv 0$. The approximation improves as more terms are included in the partial sum, and one sense in which this holds is that of a trace norm bound (see, for example, Dimassi and Sjöstrand, 1999, Theorem 9.6).

The complete asymptotic expansion by Widom (1985) can be considered a weak form of this formula (because it concerns the trace of the operator) but with discontinuities in $\boldsymbol{x}$ allowed, and extra terms exist in the expansion representing the boundary of Ω. The results by Widom (1982) and Sobolev (2013, 2015) could also be considered generalisations of this with discontinuities allowed in $\boldsymbol{x}$ and ξ. Indeed for the non self-adjoint case they imply (using the cyclic property of trace to put the operator in this form)

$$\operatorname{tr} f\big(\mathrm{op}_h^1[p(\boldsymbol{x},\xi)\chi_{\Omega\times\Lambda}(\boldsymbol{x},\xi)]\big) = \frac{1}{h^d}A_0 - \frac{\log h}{h^{d-1}}B + o\left(\frac{\log h}{h^{d-1}}\right).$$

This raises some natural questions, including:

- Does a similar result hold if we remove the condition that the discontinuity to be in $\boldsymbol{x}$ and ξ separately, instead allowing it to be an arbitrary surface in $\mathbb{R}^{2d}$?
- Does a similar result hold for other quantisations, especially the Weyl quantisation (for which $\mathrm{op}_h^{\mathrm{W}}[\chi_\Omega]$ is a self-adjoint operator)?

However, if a symbol has a discontinuity that is not just in $\boldsymbol{x}$ and ξ separately, it is not even known whether the left operator is trace class. For the Weyl quantisation the situation is even more severe: a self-adjoint operator is only trace class if it has continuous Weyl symbol. This was proved by Ramanathan and Topiwala (1993, Proposition 11) and may have been known earlier because very similar variations of this fact had already been published (for example, Grossmann, Loupias and Stein, 1968, §6). It is still possible to make sense of these questions by using a non-classical definition of operator trace (see for example Du and Wong, 2000), or by only considering f such that $f(t) = f'(t) = 0$, which ensures that the function of the operator is trace class regardless of whether the original operator is (so long as the symbol is compactly supported). But finding the answers to these questions remains difficult because the standard techniques do not apply, since they rely on the operator being trace class in the classical sense.

The main result of this thesis is a Szegő theorem where the discontinuity is not restricted to being in the two variables $\boldsymbol{x}$ and ξ separately. However, a much more tractable quantisation is used, that of *generalised anti-Wick operators*, which are discussed in the next section.

1.4 Generalised anti-Wick operators

Pseudodifferential operators, discussed in the previous section, could be intuitively viewed as the process of multiplying the time–frequency representation of a function by the symbol. Generalised anti-Wick operators have the same interpretation, but the time–frequency representation is realised as the short-time Fourier transform, which is defined for a given window function $\varphi \in L^2(\mathbb{R}^d)$ as

$$\mathscr{F}_\varphi \colon L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^{2d}), \qquad \mathscr{F}_\varphi u(\boldsymbol{s}, \xi) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi}\, u(\boldsymbol{y}) \overline{\varphi(\boldsymbol{y}-\boldsymbol{s})}\, \mathrm{d}\boldsymbol{y};$$

see for example the book by Gröchenig (2001, Chapter 3). The adjoint operator is

$$\mathscr{F}_\varphi^* \colon L^2(\mathbb{R}^{2d}) \to L^2(\mathbb{R}^d), \qquad \mathscr{F}_\varphi^* v(\boldsymbol{x}) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\xi}\, v(\boldsymbol{s}, \xi) \varphi(\boldsymbol{x}-\boldsymbol{s})\, \mathrm{d}\boldsymbol{s}\, \mathrm{d}\xi.$$

Explicitly, the *generalised anti-Wick operator* with symbol a and windows φ_1, φ_2 is

$$\mathscr{A}_{\varphi_2,\varphi_1}[a] := \mathscr{F}_{\varphi_2}^* a \mathscr{F}_{\varphi_1}.$$

These operators have the advantage of being more tractable than traditional pseudodifferential operators, but have the disadvantage that in some senses they are less "precise". For example, if a symbol $a(\boldsymbol{x})$ depends only on $\boldsymbol{x}$ (not ξ), then $\mathrm{op}_1^\tau[a]$ is just multiplication by a, but $\mathscr{A}_{\varphi_2,\varphi_1}[a]$ is multiplication by $(\varphi_2\overline{\varphi}_1)*a$.

These operators are known under several names, including Gabor–Toeplitz operators, short-time Fourier transform multipliers and time–frequency localization operators. The case where $\varphi_1 = \varphi_2$ is most often of interest, in which case we simply denote the window φ and denote the operator $\mathscr{A}_\varphi[a]$. When the window is the appropriately scaled Gaussian (see Lemma 5.5.1), the operator $\mathscr{F}_\varphi$ is also known as the *Fourier–Bros–Iagolnitzer transform* (see for example Martinez, 2001, §3.1) and the operator $\mathscr{A}_\varphi[a]$ is simply known as an *anti-Wick operator*.

As with Toeplitz operators and semiclassical pseudodifferential operators, it is of interest to determine the properties of eigenvalues when the symbol's domain is scaled up by a large factor (which we have so far denoted α or $1/h$). For a symbol $a(\boldsymbol{x},\xi)$, in §1.2 the scaling was taken on $\boldsymbol{x}$, and in §1.3 it was taken on ξ. The transformation between these choices is unitary, so the choice is not mathematically important. But in the results that follow there is little distinction made between $\boldsymbol{x}$ and ξ, so it is natural to distribute the scaling parameter over both of them. That is, we are interested in

$$\mathscr{A}_{\varphi_2,\varphi_1}[a_r] \text{ as } r \to \infty, \qquad \text{where } a_r(\boldsymbol{z}) := a(\boldsymbol{z}/r),$$

with r^2 corresponding to α and $1/h$.

Anti-Wick operators were first studied systematically by Berezin (1971). This included the first asymptotic result (Theorem 12 of that paper) about the eigenvalue counting function, in roughly the inverse situation to the one of interest here: he considered the count of eigenvalues below a fixed value, for symbols that are bounded below by a positive value.

Anti-Wick operators were later introduced to the time–frequency community by Daubechies (1988), which she called *time–frequency localization operators* when the symbol is an indicator function. This article included two asymptotic terms of the eigenvalue counting function (Remark 2 and Remark 3 in §IV.B of that paper) for a specific operator: the anti-Wick operator whose symbol is the indicator function of the unit disc D. That is, she showed that for $0 < \delta < 1$,

$$N\Big(\mathscr{A}_\varphi[\chi_{rD}], [\delta,\infty]\Big) = \frac{r^2}{2\pi}\mu_2(D) - \frac{r}{2\pi}\mu_1(\partial D)Q^{-1}(\delta) + O(1),$$

where Q is the antiderivative of the Gaussian function (i.e. the Gaussian cumulative distribution function). She proved this by explicitly finding the eigenvalues and eigenfunctions of this operator, using the fact that these are known for Weyl pseudodifferential operators with spherically symmetric symbols.

Until the work presented in this thesis, apart from the one particular case found by Daubechies, results about the eigenvalue counting function were restricted to one explicit term. The first such result for general symbols was found in one dimension by Ramanathan and Topiwala (1994, Theorem 2 and Corollary 1), and in higher dimensions by Feichtinger and Nowak (2001, Corollary 2.3 and Comment (iii) in §2), with a leading term equal to $r^{2d}\mu_{2d}(\Omega)/(2\pi)^d$ and the remainder bounded above so that it is $O(r^{2d-1})$. De Mari, Feichtinger and Nowak (2002, Example (a) on p. 731) showed that r^{2d-1} is the correct asymptotic form for the second term by also finding a lower bound for it. These authors used the term *Gabor–Toeplitz operators* for these operators.

A one-term Szegő theorem was found by Feichtinger and Nowak (2001, Theorem 2.1). The regularity requirements for that theorem are very mild: the symbol a merely has to be in $L^1 \cap L^\infty$, rather than possessing a discontinuity of the specific form χ_Ω, and the window function merely has to be in $L^2(\mathbb{R}^d)$. However, the symbol must also be positive and the two windows must be equal, which implies that the operator is positive. The result says that for sufficiently regular f satisfying $f(0)=0$ we have

$$\operatorname{tr} f\big(\mathscr{A}_\varphi[a(\boldsymbol{z}/r)]\big) = \frac{r^{2d}}{(2\pi)^d} \int_{\mathbb{R}^{2d}} f(a(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} + o(r^{2d}).$$

The result proved in this thesis is a two-term Szegő theorem for generalised anti-Wick operators. The full requirements are stated later, but the most important ones are that the windows are in the Schwartz space $\mathscr{S}(\mathbb{R}^d)$ and either Ω has C^2 boundary or it is compact with Lipschitz and piecewise C^2 boundary. For sufficiently regular f satisfying $f(0)=0$ we then have

$$\operatorname{tr} f\big(\mathscr{A}_{\varphi_2,\varphi_1}[p_r]\big) = r^{2d} A_0 + r^{2d-1} A_1 + O(r^{2d-2}),$$

as $r \to \infty$, where $p_r(\boldsymbol{z}) := a(\boldsymbol{z}/r)\chi_\Omega(\boldsymbol{z}/r)$ and

$$\begin{aligned} A_0 &= \frac{1}{(2\pi)^d} \int_\Omega f(a(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z}, \\ A_1 &= \frac{1}{(2\pi)^d} \int_{\partial\Omega} \int_{\mathbb{R}} \Big(f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) a(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) f(a(\boldsymbol{u})) \Big) \mathrm{d}\lambda\, \mu_{2d-1}(\mathrm{d}\boldsymbol{u}). \end{aligned}$$

The expression $\boldsymbol{n}(\boldsymbol{u})$ denotes the inward unit normal vector field on $\partial\Omega$. The function $Q_{\boldsymbol{\omega}}$ for $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$ will be defined in §5.2 and more information given in Lemma 5.4.2; roughly speaking, it is the function $\varphi_2\overline{\varphi_1}$ integrated in phase space in the $\boldsymbol{\omega}$ direction. It is noteworthy that there is an additional r^{2d-1} term compared to the Szegő theorem for pseudodifferential operators, but even where the boundary of Ω is not smooth there is no $r^{2d-2}\log r$ term for the "corners".

As is common, the class of allowable functions is restricted when the operator is not self-adjoint: when a is real-valued and $\varphi_1 = \varphi_2$ we require that $f \in C^\infty(\mathbb{R})$, otherwise f must be analytic. If $\inf a > -1$ then we may take $f(t) = \log(1+t)$, giving a direct analogue of the traditional Szegő theorems. Finally, if $a \equiv 1$ then the result holds with $f = \chi_{[\delta,\infty)}$, giving the eigenvalue counting function, with

$$N\Big(\mathscr{A}_\varphi[\chi_\Omega], [\delta,\infty)\Big) = \frac{r^{2d}}{(2\pi)^d}\mu_{2d}(\Omega) - \frac{r^{2d-1}}{(2\pi)^d} \int_{\partial\Omega} Q^{-1}_{\boldsymbol{n}(\boldsymbol{u})}(\delta)\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}) + o(r^{2d-1}).$$

The first term of this expansion shows how many eigenvalues are close to 1, and the second term shows how many eigenvalues are between 0 and 1 (in what is sometimes called the "plunge region"). This gives some quantitative detail to the idea that $\mathscr{A}_\varphi[\chi_\Omega]$ acts somewhat like a projection, in that it "projects" the time-frequency representation of functions on to Ω.

In fact the theorem will be proved for an even more general class of operators: Weyl pseudodifferential operators with convolution-type symbols, which are discussed in the next section.

1.5 Convolution-type symbols

The main result of this thesis — the Szegő theorem discussed at the end of the previous section — applies to an even wider class of operators than generalised anti-Wick operators. It applies to operators of the form

$$\mathrm{op}_1^{\mathrm{W}}[W * p_r] \qquad \text{where } p_r(\boldsymbol{z}) := a(\boldsymbol{z}/r)\chi_\Omega(\boldsymbol{z}/r).$$

As before, we have a symbol p_r that has a discontinuity along $\partial\Omega$ and is scaled by r, but we now apply a smooth unscaled convolution factor W and use this in the Weyl quantisation. This is a generalisation because all generalised anti-Wick operators can be written in terms of convolution and the Weyl quantisation, in which case the convolution factor W depends on the windows; this is described in §5.4.

The Szegő theorem for these operators takes the same form as for generalised anti-Wick operators, except that $Q_{\boldsymbol{\omega}}$ now depends on W rather than the window functions. The eigenvalue counting function corollary also holds, but the expression for the second term A_1 is a little more complicated than described above (unless a certain condition is satisfied; see Remark 5.3.2). There is some general interest in operators of this form (e.g. Heil, Ramanathan and Topiwala, 1995), but the main use in writing the theorem this way is that it clarifies what is really needed from the operator, and allows the proof to proceed without being distracted by the specific form of W.

In this thesis we also show a Szegő theorem for these operators where $\partial\Omega$ contains a cusp (and so is not Lipschitz). Some quite restrictive conditions are assumed, including that $f(t) = t^2$ and $d = 1$, although some of these could no doubt be relaxed. The result is then

$$f\big(\mathrm{op}_1^{\mathrm{W}}[W * p_r]\big) = r^2 A_0 + r A_1 + \Theta\big(r\,\omega^{-1}(1/r)\big),$$

where ω is a function that describes the shape of the cusp and Θ is an asymptotic notation that indicates a lower bound as well as an upper bound (see §5.6 for details). This remainder is larger than in the main result, so this shows that the Lipschitz condition could not be removed without weakening the conclusion.

There are two parts to the proof of the main Szegő theorem. The first is the composition step, where we prove

$$f\big(\mathrm{op}_1^{\mathrm{W}}[W * p_r]\big) \approx \mathrm{op}_1^{\mathrm{W}}\big[f(W * p_r)\big]$$

in the sense that the trace norm of the difference has the desired asymptotic properties. The Weyl symbol $W * p_r$ is smooth even though p is discontinuous, so we will be able to use ideas from the standard theory of Weyl pseudodifferential operators. However, the remainder is not usually bounded in the way we will need, so the standard theory is adapted to our purposes. This is done in Chapter 2, where in Lemma 2.3.5 it is shown that we may approximate a composition of two Weyl pseudodifferential operators with a finite series, with an explicit trace norm bound of the remainder expressed using the symbols in a similar way to the first excluded term. Then in Chapter 3, specifically in Lemma 3.4.3, this approximation result is extended from the composition of two operators to more general functions of an operator.

The second step of the proof is the trace asymptotics, where we show that the integral resulting from the trace of $\mathrm{op}_1^{\mathrm{W}}\big[f(W * p_r)\big]$ satisfies the required asymptotic form. This mostly consists of manipulation of geometric quantities in the immediate neighbourhood of $\partial\Omega$, for which we will need much standard theory (and a little non-standard theory) of tubular neighbourhoods, which is developed in Chapter 4. This is similar in spirit to the use of tubular neighbourhood theory by Roccaforte (1984, 2013) to find a geometrical interpretation for terms in the Szegő expansion for truncated Wiener–Hopf operators.

Chapter 5 contains the precise statement of the result. This includes both the Szegő theorem (§5.2) and the eigenvalue counting function (§5.3) in their general form, and a description of how they apply to generalised anti-Wick operators (§5.4), along with the cusp result (§5.6). There is an overview of the idea of the proof of the main result (§5.7), while the full proof is given in Chapter 6.

Chapter 2

Pseudodifferential operator composition

This chapter is concerned with approximating the composition of two pseudodifferential operators by a single pseudodifferential operator with the product of symbols; that is,

$$\mathrm{op}[p]\,\mathrm{op}[q] \approx \mathrm{op}[pq].$$

This will be used in Chapter 3 to gain information about $f(\mathrm{op}[q])$.

In fact we may improve the right hand side of the above equation by approximating the symbol of composition by an infinite series, with pq for the first term and with derivatives of p and q in higher terms. There are several senses in which such a series can be considered as approximating the composition:

1. We may define pseudodifferential operator symbol classes, such as the Hörmander classes or Shubin classes. These classes depend on a number $n \in \mathbb{R}$ and are defined in such a way that a differential operator of order n is in the class of order n. Asymptotic series then consist of terms in symbol classes of decreasing order.

2. We may consider the semiclassical operators, whose symbols are dilated by a parameter h considered asymptotically as $h \to 0$. In this case the j^{th} term in a series is, roughly speaking, required to be of size h^j.

3. The sense that will be important in this document is that if p and q are convolution-type as discussed in §1.5 then we wish the error in approximation to have a trace norm bounded by a sufficiently low power of r.

We will start, in §2.1, by giving a precise definition of pseudodifferential operators and recalling some standard properties that we will need later. In §2.2 we cover some technicalities regarding integrals of functions of an oscillating character. In §2.3 we will give the key result of this chapter: a bound for the trace norm and operator norm of the remainder of approximating the composition of two Weyl pseudodifferential operators by the partial sum of the series expansion. These bounds are just directly expressed in terms of the Weyl symbols, rather than being defined in some presupposed sense as in the list above. In fact we will only need first term of the series, and only the trace norm bound, but the general result is no harder to prove and of general interest. The techniques more usually used to prove asymptotic composition results are outlined in §2.4, and later, in §5.7, these will be compared with the ideas used in this thesis.

2.1 Trace norm and operator norm bounds

In this section we will define pseudodifferential operators and give their basic properties, including bounds on their operator norms and trace norms in terms of their symbols. As always where the Fourier transform is involved, there are several conventions in common use differing only by scaling and multiplicative factors; here we follow the convention used, for example, by Martinez (2001, Definition 2.5.1).

To simplify the exposition, in this thesis we will only consider symbols belonging to the set

$$C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d}) := \{q \in L^{\infty}(\mathbb{R}^{2d}) \mid \forall \alpha \in \mathbb{N}_0^{2d} : \partial^{\alpha} q \in L^{\infty}(\mathbb{R}^{2d})\}.$$

(Here the set of natural numbers including zero is denoted by $\mathbb{N}_0$, so that the set of m-dimensional multi-indices is $\mathbb{N}_0^m$.) In other words, $C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ is the space of bounded complex-valued functions on $\mathbb{R}^{2d}$ that are infinitely differentiable and whose derivatives are all bounded (but not necessarily all bounded by the same value). This set is sometimes denoted $C^{\infty}(\mathbb{R}^{2d})$, but here, as is common elsewhere, that notation is used instead to refer to all functions that are merely infinitely differentiable with no boundedness requirement; in this respect we are following the notation of Shubin (2001, §23.2).

Definition 2.1.1. For $q \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ and $\tau \in [0,1]$ we define the operator $\mathrm{op}_1^{\tau}[q] \colon \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ by

$$\mathrm{op}_1^{\tau}[q]u(\boldsymbol{x}) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi} q\big(\tau\boldsymbol{x} + (1-\tau)\boldsymbol{y}, \xi\big) u(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y} \,\mathrm{d}\xi.$$

This is to be understood as an iterated integral. The integrand is absolutely integrable in $\boldsymbol{y}$ because u is integrable and q is bounded; indeed the product is a Schwartz function in $\boldsymbol{y}$. It is a simple and standard fact that the Fourier transform of a Schwartz function is again Schwartz, and in the same way the inner integral is a Schwartz function of ξ, as is the outer integral as a function of $\boldsymbol{x}$; see Lemma 2.2.5 for full details.

The subscript 1 in op_1^{τ} denotes the value of the semiclassical parameter h. We will define the operator with general semiclassical parameter in Notation 2.4.9. From this point onwards we will usually work with the Weyl quantisation, which we denote

$$\mathrm{op}_h^{\mathrm{W}}[q] := \mathrm{op}_h^{1/2}[q].$$

We rarely use the semiclassical parameter, so we usually use the even briefer notation

$$\mathrm{op}[q] := \mathrm{op}_1^{1/2}[q].$$

Definition 2.1.1 is very explicit and therefore useful for calculating properties of $\mathrm{op}_1^\tau[q]$, but the operator of interest here is the one acting on $L^2(\mathbb{R}^d)$ rather than the one acting on $\mathscr{S}(\mathbb{R}^d)$. That is defined by the density of Schwartz functions in $L^2(\mathbb{R}^d)$, and is expressed in the following lemma.

Lemma 2.1.2. *Let $q \in C_\mathrm{b}^\infty(\mathbb{R}^{2d})$. Then $\mathrm{op}_1^\tau[q]$ extends uniquely from an operator $\mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ to a bounded operator $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. There exist constants $C_{d,\tau}$ and $C'_{d,\tau}$, independent of q, such that the operator norm of this operator satisfies*

$$\|\mathrm{op}_1^\tau[q]\| \leqslant C_{d,\tau} \max_{|\boldsymbol{k}| \leqslant C'_{d,\tau}} \|\partial^{\boldsymbol{k}} q\|_{L^\infty(\mathbb{R}^{2d})},$$

In the case that $\tau = \frac{1}{2}$ (the Weyl quantisation), this inequality holds with $C'_{d,1/2} = d+2$.

Calderón and Vaillancourt (1971) first proved this for the left quantisation ($\tau = 1$), and later they proved a much more general result (Calderón and Vaillancourt, 1972) that includes the above statements for general τ (apart from the final statement about $C'_{d,1/2}$). Since then there have been improvements to the constant $C'_{d,\tau}$, including a result for the Weyl quantisation by Boulkhemair (1999), which says

$$\|\mathrm{op}[q]\| \leqslant C_{d,1/2} \max_{\substack{|\boldsymbol{k}_1| \leqslant \lfloor d/2 \rfloor + 1 \\ |\boldsymbol{k}_2| \leqslant \lfloor d/2 \rfloor + 1}} \|\partial_{\boldsymbol{x}}^{\boldsymbol{k}_1} \partial_\xi^{\boldsymbol{k}_2} q(\boldsymbol{x}, \xi)\|_{L^\infty(\mathbb{R}^{2d})},$$

which implies the final statement in the lemma.

Other properties of pseudodifferential operators are that $\mathrm{op}_1^\tau[0]$ is the zero operator, $\mathrm{op}_1^\tau[1]$ is the identity operator, and that the adjoint is given by

$$(\mathrm{op}_1^\tau[q])^* = \mathrm{op}_1^{1-\tau}[\overline{q}];$$

note that when $\tau = \frac{1}{2}$ both sides of this identity are the Weyl quantisation. We also have the rescaling property that for any $\lambda > 0$ there is the unitary equivalence

$$\mathrm{op}_1^\tau[q(\boldsymbol{x}, \xi)] \cong \mathrm{op}_1^\tau[q(\boldsymbol{x}/\lambda, \lambda\xi)].$$

For these and other basic properties, the reader is referred to any of the many excellent texts on the subject; for example, the books by Folland (1989, Chapter 2) and Shubin (2001, Chapter IV).

We will also need facts about the trace and trace norm of pseudodifferential operators. For an operator A, we denote the trace by $\operatorname{tr} A$ and the trace norm by $\|A\|_1$; see for example Birman and Solomjak (1987, §11.2) for their definitions. The main result of this thesis is about the trace of an operator, so we will need a formula for this in terms of the operator's Weyl symbol. This also requires that we bound the trace norm, for two reasons. First, the trace of an operator is only well defined when it has finite trace norm. Second, we will often want to bound the trace of the composition of two operators, which can be done by combining the general facts

$$\|AB\|_1 \leqslant \|A\|_1 \|B\|, \qquad |\operatorname{tr} C| \leqslant \|C\|_1,$$

which hold for all trace class A and C and bounded B (see Birman and Solomjak, 1987, §11.2). The following lemma expresses the trace formula and a trace class bound for Weyl pseudodifferential operators.

Lemma 2.1.3. *Let $q \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$. Then there exists a constant C_d independent of q such that the trace norm of* $\mathrm{op}[q]$ *satisfies*

$$\|\mathrm{op}[q]\|_1 \leqslant C_d \sum_{|\boldsymbol{k}| \leqslant 2d+1} \|\partial^{\boldsymbol{k}} q\|_{L^1(\mathbb{R}^{2d})}.$$

In particular, if the right hand side is finite then the operator is trace class and the trace satisfies

$$\operatorname{tr} \mathrm{op}[q] = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} q(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z}.$$

The bound on the trace norm (without specifying the number of derivatives required) was first found by Tulovsky and Shubin (1973, Theorem 4.1). Another early publication of this result was the book by Shubin (2001, Proposition 27.3), which was originally published in Russian in 1978, and includes a similar bound for all quantisations rather than just the Weyl quantisation, and is proved in rather more detail. The first publication of the trace formula is harder to establish, partly because it easily follows (at least formally) from the trace formula for integral operators so it is sometimes used without being stated explicitly or proved in full; it was certainly used at least as far back as the paper by Tulovsky and Shubin (1973, proof of Proposition 5.2). Lemma 2.1.3 as stated, including the trace formula and the bound with $2d+1$ derivatives, follows from Dimassi and Sjöstrand (1999, Theorem 9.4).

2.2 Bounds for integrals of oscillating functions

It is a standard fact that if $f \in \mathscr{S}(\mathbb{R}^d)$ then $\hat{f} \in \mathscr{S}(\mathbb{R}^d)$. This is easy to prove, with differentiation under the integral giving the smoothness and integration by parts showing that, for every $n \in \mathbb{N}_0$, we have

$$\hat{f}(\boldsymbol{x}) = O\left(\frac{1}{|\boldsymbol{x}|^n}\right) \qquad \text{as } |\boldsymbol{x}| \to \infty.$$

In this section we will prove simple variants of the latter part; we will show that integrals of suitably oscillating functions, such as $\mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\boldsymbol{\xi}} f(\boldsymbol{y})$, decay quickly at infinity, but use a bound that has no singularity at zero. Everything in this section is standard, but we will need to apply these techniques later so it is helpful to isolate them here from the novel material. To express the results neatly we will use the following common convention.

Definition 2.2.1. For any $\boldsymbol{x} \in \mathbb{R}^m$, we set

$$\langle \boldsymbol{x} \rangle := (1 + |\boldsymbol{x}|^2)^{1/2}.$$

This is a smooth function $\mathbb{R}^m \to [1, \infty)$, with $\langle \boldsymbol{x} \rangle \geqslant 1$ and $\langle \boldsymbol{x} \rangle \geqslant |\boldsymbol{x}|$ for $\boldsymbol{x} \in \mathbb{R}^m$, and $\langle \boldsymbol{x} \rangle \leqslant \sqrt{2}|\boldsymbol{x}|$ for $|\boldsymbol{x}| \geqslant 1$ (because $1+|\boldsymbol{x}|^2 \leqslant 2|\boldsymbol{x}|^2$). It also satisfies the useful relationship given in the next lemma.

Lemma 2.2.2. *If $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^m$ then*

$$\langle \boldsymbol{x} + \boldsymbol{y} \rangle \leqslant \sqrt{2} \langle \boldsymbol{x} \rangle \langle \boldsymbol{y} \rangle.$$

Proof. We have

$$\begin{aligned}
\langle \boldsymbol{x} + \boldsymbol{y} \rangle^2 &= 1 + |\boldsymbol{x} + \boldsymbol{y}|^2 \leqslant 1 + (|\boldsymbol{x}| + |\boldsymbol{y}|)^2 = 1 + |\boldsymbol{x}|^2 + 2|\boldsymbol{x}||\boldsymbol{y}| + |\boldsymbol{y}|^2, \\
\langle \boldsymbol{x} \rangle^2 \langle \boldsymbol{y} \rangle^2 &= (1 + |\boldsymbol{x}|^2)(1 + |\boldsymbol{y}|^2) = 1 + |\boldsymbol{x}|^2 + |\boldsymbol{y}|^2 + |\boldsymbol{x}|^2 |\boldsymbol{y}|^2,
\end{aligned}$$

so

$$\begin{aligned}
2\langle \boldsymbol{x} \rangle^2 \langle \boldsymbol{y} \rangle^2 - \langle \boldsymbol{x} + \boldsymbol{y} \rangle^2 &\geqslant 2|\boldsymbol{x}|^2 |\boldsymbol{y}|^2 + |\boldsymbol{x}|^2 + |\boldsymbol{y}|^2 + 1 - 2|\boldsymbol{x}||\boldsymbol{y}| \\
&\geqslant |\boldsymbol{x}|^2 |\boldsymbol{y}|^2 - 2|\boldsymbol{x}||\boldsymbol{y}| + 1 = (|\boldsymbol{x}||\boldsymbol{y}| - 1)^2 \geqslant 0.
\end{aligned}$$

This proves the inequality. □

The quantity $\langle \boldsymbol{x} \rangle$ is also useful for bounding functions asymptotically, because for any $n \in \mathbb{N}_0$ it satisfies

$$f(\boldsymbol{x}) = O\left(\frac{1}{|\boldsymbol{x}|^n}\right) \quad \Longleftrightarrow \quad f(\boldsymbol{x}) = O\left(\frac{1}{\langle \boldsymbol{x} \rangle^n}\right)$$

as $|\boldsymbol{x}| \to \infty$. To prove bounds in terms of $1/\langle \boldsymbol{x} \rangle^n$, we will often integrate by parts with the following differential operator, as is done, for example, in Martinez (2001, comments after Theorem 2.4.1). In effect, using it to bound an integral is like integrating by parts for $|\xi| > 1$ and separately bounding the integral for $|\xi| < 1$, but with a smooth transition (allowing the derivative in $\boldsymbol{x}$ in Lemma 2.2.4).

Notation 2.2.3. We define

$$P_{\boldsymbol{y},\xi} := \frac{1 + \mathrm{i}\xi \cdot \nabla_{\boldsymbol{y}}}{\langle \xi \rangle^2}, \quad \Longrightarrow \quad P_{\boldsymbol{y},\xi}^{\mathrm{T}} = \frac{1 - \mathrm{i}\xi \cdot \nabla_{\boldsymbol{y}}}{\langle \xi \rangle^2}.$$

In particular, $P_{\boldsymbol{y},\xi} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} = \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi}$. We may write $(P_{\boldsymbol{y},\xi})^n$ in terms of multi-indices by applying the binomial theorem and multinomial theorem, so that for any $n \in \mathbb{N}_0$ we have

$$(P_{\boldsymbol{y},\xi})^n = \sum_{r=0}^{n} \binom{n}{r} \frac{(\mathrm{i}\xi \cdot \nabla_{\boldsymbol{y}})^r}{\langle \xi \rangle^{2n}}, \qquad (\mathrm{i}\xi \cdot \nabla_{\boldsymbol{y}})^r = \mathrm{i}^r \sum_{|\boldsymbol{\alpha}|=r} \binom{r}{\boldsymbol{\alpha}} \xi^{\boldsymbol{\alpha}} \partial_{\boldsymbol{y}}^{\boldsymbol{\alpha}},$$

giving

$$(P_{\boldsymbol{y},\xi})^n = \sum_{|\boldsymbol{\alpha}| \leqslant n} \binom{n}{|\boldsymbol{\alpha}|} \binom{|\boldsymbol{\alpha}|}{\boldsymbol{\alpha}} \frac{\mathrm{i}^{|\boldsymbol{\alpha}|} \xi^{\boldsymbol{\alpha}} \partial_{\boldsymbol{y}}^{\boldsymbol{\alpha}}}{\langle \xi \rangle^{2n}}.$$

The next lemma, most often applied with $\boldsymbol{a} = \mathbf{0}$ (i.e. no derivatives), shows that integrating by parts with $P_{\boldsymbol{y},\boldsymbol{\xi}}$ gives the required decay despite the presence of positive powers of $\boldsymbol{\xi}$ in the numerator of $(P_{\boldsymbol{y},\boldsymbol{\xi}})^n$.

Lemma 2.2.4. *Let $\boldsymbol{a},\boldsymbol{k} \in \mathbb{N}_0^d$ and $Q \in \mathbb{N}$ such that $|\boldsymbol{k}| \leqslant Q$. Then there exists a constant $C_{\boldsymbol{a},Q}$ such that*

$$\left|\partial_{\boldsymbol{x}}^{\boldsymbol{a}} \frac{\boldsymbol{x}^{\boldsymbol{k}}}{\langle \boldsymbol{x}\rangle^{2Q}}\right| \leqslant C_{\boldsymbol{a},Q} \frac{1}{\langle \boldsymbol{x}\rangle^{Q}}.$$

Proof. For any $r \in \mathbb{N}$, $\boldsymbol{l} \in \mathbb{N}_0^d$ such that $|\boldsymbol{l}| \leqslant r$, let

$$F_{\boldsymbol{l},r}(\boldsymbol{x}) := \frac{\boldsymbol{x}^{\boldsymbol{l}}}{\langle \boldsymbol{x}\rangle^{Q+r}}.$$

We will show that the left hand side of the inequality is a sum of terms of the form $F_{\boldsymbol{l},r}$, and by bounding the terms and their coefficients the result follows.

Bound for $F_{\boldsymbol{l},r}$. We have

$$|F_{\boldsymbol{l},r}(\boldsymbol{x})| \leqslant \left|\frac{\boldsymbol{x}^{\boldsymbol{l}}}{\langle \boldsymbol{x}\rangle^{Q+r}}\right| \leqslant \frac{\langle \boldsymbol{x}\rangle^{|\boldsymbol{l}|}}{\langle \boldsymbol{x}\rangle^{Q+r}} \leqslant \frac{1}{\langle \boldsymbol{x}\rangle^{Q}}.$$

Derivative of $F_{\boldsymbol{l},r}$. Let $n \leqslant d$ and let $\hat{\boldsymbol{n}}$ be the multi-index with 1 in the n^{th} place and zeros in the other places. First observe that for any $p \in \mathbb{N}_0$ we have

$$\partial_{x_n} \frac{1}{\langle \boldsymbol{x}\rangle^{p}} = \partial_{x_n} \frac{1}{(1+x_1^2+\cdots+x_d^2)^{p/2}} = 2x_n \frac{-p/2}{(1+x_1^2+\cdots+x_d^2)^{p/2+1}} = -p\frac{\boldsymbol{x}^{\hat{\boldsymbol{n}}}}{\langle \boldsymbol{x}\rangle^{p+2}}.$$

Thus

$$\partial_{x_n} F_{\boldsymbol{l},r}(\boldsymbol{x}) = \partial_{x_n} \frac{\boldsymbol{x}^{\boldsymbol{l}}}{\langle \boldsymbol{x}\rangle^{Q+r}} = \begin{cases} l_n \dfrac{\boldsymbol{x}^{\boldsymbol{l}-\hat{\boldsymbol{n}}}}{\langle \boldsymbol{x}\rangle^{Q+r}} - (Q+r)\dfrac{\boldsymbol{x}^{\boldsymbol{l}+\hat{\boldsymbol{n}}}}{\langle \boldsymbol{x}\rangle^{Q+r+2}} & \text{if } l_n > 0, \\ -(Q+r)\dfrac{\boldsymbol{x}^{\boldsymbol{l}+\hat{\boldsymbol{n}}}}{\langle \boldsymbol{x}\rangle^{Q+r+2}} & \text{if } l_n = 0. \end{cases}$$

Note that this is the weighted sum of one or two terms also of the form $F_{\boldsymbol{l},r}$.

Conclusion. We have

$$\frac{\boldsymbol{x}^{\boldsymbol{k}}}{\langle \boldsymbol{x}\rangle^{2Q}} = F_{\boldsymbol{k},Q}(\boldsymbol{x}),$$

so $\partial_{\boldsymbol{x}}^{\boldsymbol{a}}\big(\boldsymbol{x}^{\boldsymbol{k}}/\langle \boldsymbol{x}\rangle^{2Q}\big)$ is a sum of such terms. For each term, r is at most $Q+2|\boldsymbol{a}|$ and l_n is at most $|\boldsymbol{k}|+|\boldsymbol{a}|$, so the coefficients are bounded by

$$\max\{Q+Q+2|\boldsymbol{a}|, |\boldsymbol{k}|+|\boldsymbol{a}|\}^{|\boldsymbol{a}|} = (2(Q+|\boldsymbol{a}|))^{|\boldsymbol{a}|}.$$

There are at most $2^{|\boldsymbol{a}|}$ of these terms, so the result holds with $C_{\boldsymbol{a},Q} = (4(Q+|\boldsymbol{a}|))^{|\boldsymbol{a}|}$. □

An example application of $P_{\boldsymbol{y},\boldsymbol{\xi}}$ and Lemma 2.2.4 to obtain decay is the next lemma, which shows that the pseudodifferential operators as defined in Definition 2.1.1 map $\mathscr{S}(\mathbb{R}^d)$ into itself as claimed.

Lemma 2.2.5. *Let $p \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{3d})$ and $u \in \mathscr{S}(\mathbb{R}^d)$. Then the following all hold:*

1. *For each $\boldsymbol{x}, \xi \in \mathbb{R}^d$ we have $\big(\boldsymbol{y} \mapsto p(\boldsymbol{x},\boldsymbol{y},\xi)u(\boldsymbol{y})\big) \in \mathscr{S}(\mathbb{R}^d)$.*
2. *For each $\boldsymbol{x} \in \mathbb{R}^d$ we have $\big(\xi \mapsto \int \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} p(\boldsymbol{x},\boldsymbol{y},\xi)u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\big) \in \mathscr{S}(\mathbb{R}^d)$.*
3. *We have $\big(\boldsymbol{x} \mapsto \iint \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi} p(\boldsymbol{x},\boldsymbol{y},\xi)u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\xi\big) \in \mathscr{S}(\mathbb{R}^d)$.*

Proof. Statement 1. This follows immediately from the product rule and the definition of $C_{\mathrm{b}}^{\infty}(\mathbb{R}^{3d})$ and $\mathscr{S}(\mathbb{R}^d)$.

Statement 2. For any $\boldsymbol{x}, \xi \in \mathbb{R}^d$, set

$$f(\boldsymbol{x},\xi) := \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} p(\boldsymbol{x},\boldsymbol{y},\xi)u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

The first statement implies that this integral is well-defined, and that we may differentiate under the integral (see Lang, 1993, Chapter XIII, Lemma 2.2). This implies that that f is infinitely differentiable in $\boldsymbol{x}$ and ξ, and for any $\boldsymbol{a} \in \mathbb{N}_0^d$ we have

$$\begin{aligned}
\partial_{\xi}^{\boldsymbol{a}} f(\boldsymbol{x},\xi) &= \int_{\mathbb{R}^d} \partial_{\xi}^{\boldsymbol{a}}\Big(\mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} p(\boldsymbol{x},\boldsymbol{y},\xi)\Big)u(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \\
&= \sum_{\boldsymbol{b}\leqslant\boldsymbol{a}} \binom{\boldsymbol{a}}{\boldsymbol{b}} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} \underbrace{(-\mathrm{i}\boldsymbol{y})^{\boldsymbol{b}} \partial_{\xi}^{\boldsymbol{a}-\boldsymbol{b}} p(\boldsymbol{x},\boldsymbol{y},\xi)u(\boldsymbol{y})}_{=:g_{\boldsymbol{a},\boldsymbol{b}}(\boldsymbol{x},\boldsymbol{y},\xi)}\mathrm{d}\boldsymbol{y}.
\end{aligned}$$

But because $u \in \mathscr{S}(\mathbb{R}^d)$, $g_{\boldsymbol{a},\boldsymbol{b}}(\boldsymbol{x},\boldsymbol{y},\xi)$ is rapidly decaying in $\boldsymbol{y}$. It remains to show that f and its derivatives in ξ decay sufficiently quickly as $|\xi| \to \infty$, which we do by integrating by parts. Define $P_{\boldsymbol{y},\xi}$ as in Notation 2.2.3. For any $\boldsymbol{a} \in \mathbb{N}_0^d$ and $n \in \mathbb{N}_0$, applying Lemma 2.2.4 (with $\boldsymbol{a} = \boldsymbol{0}$), we have

$$\begin{aligned}
|\partial_{\xi}^{\boldsymbol{a}} f(\boldsymbol{x},\xi)| &\leqslant \sum_{\boldsymbol{b}\leqslant\boldsymbol{a}} \binom{\boldsymbol{a}}{\boldsymbol{b}} \left| \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} (P_{\boldsymbol{y},\xi}^{\mathrm{T}})^n g_{\boldsymbol{a},\boldsymbol{b}}(\boldsymbol{x},\boldsymbol{y},\xi)\,\mathrm{d}\boldsymbol{y} \right| \\
&\leqslant \sum_{\boldsymbol{b}\leqslant\boldsymbol{a}} \binom{\boldsymbol{a}}{\boldsymbol{b}} \int_{\mathbb{R}^d} C_{\boldsymbol{a},\boldsymbol{b}} \frac{1}{\langle\xi\rangle^n \langle\boldsymbol{y}\rangle^{d+1}}\,\mathrm{d}\boldsymbol{y},
\end{aligned}$$

where $C_{\boldsymbol{a},\boldsymbol{b}}$ is a value not dependent on $\boldsymbol{x}$, $\boldsymbol{y}$ or ξ (but is dependent on p and u); thus $\partial^{\boldsymbol{a}} f(\xi)$ is bounded by any inverse power of $\langle\xi\rangle$.

Statement 3. We will need two observations about the statement 2. First, the bound we obtained for $\partial_{\xi}^{\boldsymbol{a}} f(\boldsymbol{x},\xi)$ was uniform in $\boldsymbol{x}$ (due to our assumption about the boundedness of derivatives of p). The other is that we may differentiate f by $\boldsymbol{x}$ under the integral, and by the exactly the same logic as above (with $\partial_{\boldsymbol{x}}^{\boldsymbol{c}} p$ in place of p) we find that $\partial_{\boldsymbol{x}}^{\boldsymbol{c}} \partial_{\xi}^{\boldsymbol{a}} f(\boldsymbol{x},\xi)$ is also bounded by a constant multiple of $1/\langle\xi\rangle^n$ uniformly in $\boldsymbol{x}$. Then statement 3 follows in the same way as the statement 2, integrating by parts in the $\mathrm{d}\xi$ integral this time rather than the $\mathrm{d}\boldsymbol{y}$ integral. To be explicit, set

$$h(\boldsymbol{x}) := \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\xi} f(\boldsymbol{x},\xi)\,\mathrm{d}\xi.$$

Working in the same way as before, we have

$$\begin{aligned}|\partial^{\boldsymbol{a}} h(\boldsymbol{x})| &\leqslant \sum_{\boldsymbol{b}\leqslant\boldsymbol{a}} \binom{\boldsymbol{a}}{\boldsymbol{b}} \left| \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\xi} (P_{\xi,\boldsymbol{x}})^n f(\boldsymbol{x},\xi)\,\mathrm{d}\xi \right| \\ &\leqslant \sum_{\boldsymbol{b}\leqslant\boldsymbol{a}} \binom{\boldsymbol{a}}{\boldsymbol{b}} \int_{\mathbb{R}^d} C'_{\boldsymbol{a},\boldsymbol{b}} \frac{1}{\langle\boldsymbol{x}\rangle^n \langle\xi\rangle^{d+1}} \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\xi} (P_{\xi,\boldsymbol{x}})^n f(\boldsymbol{x},\xi)\,\mathrm{d}\xi.\end{aligned}$$

Thus $\partial^{\boldsymbol{a}} h(\boldsymbol{x})$ is bounded by any inverse power of $\langle\boldsymbol{x}\rangle$. □

2.3 Composition with explicit remainder

In this section we approximate the composition of two operators by a finite series expressed in terms of the Weyl symbols of the original operators, with explicit trace norm and operator norm bounds on the remainder. The initial part of the discussion is standard, but by being careful when bounding the remainder we preserve cancellation that is usually lost; a comparison with the usual approach is made in §2.4.

Notation 2.3.1. When $\boldsymbol{x} \in \mathbb{R}^{2d}$, in this section we will refer to the two vector components using the notation

$$\boldsymbol{x}_1 := (x_1, \ldots, x_d) \in \mathbb{R}^d, \qquad \boldsymbol{x}_2 := (x_{d+1}, \ldots, x_{2d}) \in \mathbb{R}^d.$$

The first expression we consider for the Weyl symbol of the composition of two operators is given in the next lemma. This is proved, for example, in the book by Folland (1989, (2.44b)). The expression $p \,\#\, q$ is sometimes called the *twisted product* or *Moyal product* of p and q, and σ is the standard symplectic form on $\mathbb{R}^{2d}$.

Lemma 2.3.2. *Let $p, q \in \mathscr{S}(\mathbb{R}^{2d})$. Set*

$$p \,\#\, q(\boldsymbol{z}) := \frac{1}{\pi^{2d}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} p(\boldsymbol{z}-\boldsymbol{x}) q(\boldsymbol{z}-\boldsymbol{y}) \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}, \qquad \sigma(\boldsymbol{x},\boldsymbol{y}) := \boldsymbol{x}_1\cdot\boldsymbol{y}_2 - \boldsymbol{y}_1\cdot\boldsymbol{x}_2,$$

which in particular satisfies $p \,\#\, q \in \mathscr{S}(\mathbb{R}^{2d})$. Then

$$\mathrm{op}[p]\,\mathrm{op}[q] = \mathrm{op}[p \,\#\, q].$$

The series representation for $p \,\#\, q$ follows from this by taking the Taylor series and using the Fourier inversion theorem. It is ultimately irrelevant whether the Taylor series is taken in the $\boldsymbol{x}$ or $\boldsymbol{y}$ variable, or even in $(\boldsymbol{x}_1, \boldsymbol{y}_1)$ or $(\boldsymbol{x}_2, \boldsymbol{y}_2)$; we will work with the $\boldsymbol{x}$ variable. This is done in the next lemma, which is standard but usually not distilled out explicitly. For example, it is essentially proved by Folland (1989, Theorem (2.49)), although the remainder term is not written out there (but the analogous term is in Folland, 1989, Theorem (2.41)).

Lemma 2.3.3. *Let $p, q \in \mathscr{S}(\mathbb{R}^{2d})$ and $n \in \mathbb{N}_0$. Set*

$$F_j(\boldsymbol{x},\boldsymbol{y}) := \frac{\mathrm{i}^j}{j!2^j}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})^j(p(\boldsymbol{x})q(\boldsymbol{y})), \quad c_n(\boldsymbol{z}) := \sum_{j=0}^{n} F_j(\boldsymbol{z},\boldsymbol{z}).$$

Then

$$\mathrm{op}[p]\,\mathrm{op}[q] = \mathrm{op}[c_n] + \mathrm{op}[R_{n+1}],$$

where, setting $g_n(t) := (n+1)(1-t)^n$ so that $\int_0^1 g_n(t)\,\mathrm{d}t = 1$, we have

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}}\int_0^1\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} g_n(t)\,F_{n+1}(\boldsymbol{z}-\sqrt{t}\boldsymbol{x},\boldsymbol{z}-\sqrt{t}\boldsymbol{y})\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t.$$

Furthermore $c_n, R_{n+1} \in \mathscr{S}(\mathbb{R}^{2d})$.

Remark 2.3.4. The expression for F_j in Lemma 2.3.3 (which is used in the definition of c_n and R_{n+1}) may instead be written in terms of multi-indices, which is useful for some computations. Specifically, for any multi-index $\boldsymbol{m} \in \mathbb{N}_0^{2d}$, denote

$$\tau(\boldsymbol{m}) := (\boldsymbol{m}_2, \boldsymbol{m}_1) = (m_{d+1}, m_{d+2}, \ldots, m_{2d}, m_1, m_2, \ldots, m_d);$$

then

$$F_j(\boldsymbol{x},\boldsymbol{y}) = \frac{\mathrm{i}^j}{j!2^j}\sum_{|\boldsymbol{m}|=j}(-1)^{|\boldsymbol{m}_2|}\partial^{\boldsymbol{m}}p(\boldsymbol{x})\partial^{\tau(\boldsymbol{m})}q(\boldsymbol{y}).$$

Proof of Lemma 2.3.3. Expression for series. We apply Taylor's theorem to p. The corresponding term of $p\,\#\,q(\boldsymbol{z})$ is

$$T_j(\boldsymbol{z}) = \frac{1}{\pi^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\frac{1}{j!}(-\boldsymbol{x}\cdot\nabla_p)^j(p(\boldsymbol{z})q(\boldsymbol{z}-\boldsymbol{y}))\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x},$$

where ∇_p indicates that the gradient is being taken only of p. Denote $\widetilde{\nabla}_{\boldsymbol{y}} := (\nabla_{\boldsymbol{y}_2}, -\nabla_{\boldsymbol{y}_1})$, so that $2\mathrm{i}\boldsymbol{x}\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})} = \widetilde{\nabla}_{\boldsymbol{y}}\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}$; then integrating by parts gives

$$\begin{aligned} T_j(\boldsymbol{z}) &= \frac{1}{\pi^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\frac{\mathrm{i}^j}{j!2^j}(\nabla_p\cdot\widetilde{\nabla}_q)^j(p(\boldsymbol{z})q(\boldsymbol{z}-\boldsymbol{y}))\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x} \\ &= \frac{1}{\pi^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} F_j(\boldsymbol{z},\boldsymbol{z}-\boldsymbol{y})\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

(The sign comes from four multiples of $(-1)^j$: one from $(-\boldsymbol{x}\cdot\nabla)^j$, one from integrating by parts, one from differentiating with respect to $\boldsymbol{y}$ while q depends on $-\boldsymbol{y}$, and one from replacing $1/\mathrm{i}$ with $-\mathrm{i}$.) By the Fourier inversion theorem this equals $F_j(\boldsymbol{z},\boldsymbol{z})$.

Expression for R_{n+1}. The remainder term satisfies

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\int_0^1(1-t)^n\frac{1}{n!}(-\boldsymbol{x}\cdot\nabla_p)^{n+1}(p(\boldsymbol{z}-t\boldsymbol{x})q(\boldsymbol{z}-\boldsymbol{y}))\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}t\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}.$$

Integrating by parts in the same way as the other terms, we find that

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\int_0^1 g_n(t)\,F_{n+1}(\boldsymbol{z}-t\boldsymbol{x},\boldsymbol{z}-\boldsymbol{y})\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}t\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}.$$

We may interchange the order of integration between $\mathrm{d}t$ and $\mathrm{d}\boldsymbol{y}$ because the integrand is a Schwartz function in $\boldsymbol{y}$ uniformly in t (because F_{n+1} is Schwartz in its second variable), and it is a continuous function of t on a bounded interval, so we may apply Fubini's theorem. To interchange the order of integration between $\mathrm{d}t$ and $\mathrm{d}\boldsymbol{x}$, it is not sufficient to use the fact that F_{n+1} is Schwartz in its first variable because that does not immediately imply that the integrand is Schwartz uniformly in t. However, considering the $\mathrm{d}y$ integral as a function of $\boldsymbol{x}$ and t, applying the same reasoning as in Lemma 2.2.5 shows that this integral is Schwartz in $\boldsymbol{x}$ uniformly in t, so we may apply Fubini's theorem again to give

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t)\, F_{n+1}(\boldsymbol{z} - t\boldsymbol{x}, \boldsymbol{z} - \boldsymbol{y})\, \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\, \mathrm{d}\boldsymbol{y}\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}t.$$

Setting $\sqrt{t}\boldsymbol{x}' = t\boldsymbol{x}$ and $\sqrt{t}\boldsymbol{y}' := \boldsymbol{y}$, which satisfies $\sigma(\boldsymbol{x},\boldsymbol{y}) = \sigma(\boldsymbol{x}',\boldsymbol{y}')$ and has Jacobian 1, gives the stated result.

<u>$c_n, R_{n+1} \in \mathscr{S}(\mathbb{R}^{2d})$.</u> The function c_n is a linear combination of products of derivatives of p and q, which are Schwartz by hypothesis, so is also Schwartz. Then $R_n = p\#q - c_n$, which as the difference of Schwartz functions is also Schwartz. □

We now arrive at the promised explicit trace norm and operator norm bounds for the remainder.

Lemma 2.3.5. *Let $p, q \in \mathscr{S}(\mathbb{R}^{2d})$ and $n, G \in \mathbb{N}_0$. Define F_j and c_n as in Lemma 2.3.3. Then*

$$\|\mathrm{op}[p]\,\mathrm{op}[q] - \mathrm{op}[c_n]\|_1 \leqslant C_{d,G} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+4d+2}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z} - \frac{1}{2}\boldsymbol{v}, \boldsymbol{z} + \frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{v}\rangle^G}\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}\boldsymbol{z},$$

$$\|\mathrm{op}[p]\,\mathrm{op}[q] - \mathrm{op}[c_n]\| \leqslant C'_{d,G} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+3d+3}} \sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z} - \frac{1}{2}\boldsymbol{v}, \boldsymbol{z} + \frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{v}\rangle^G}\, \mathrm{d}\boldsymbol{v}.$$

The constants $C_{d,G}$ and $C'_{d,G}$ depend only on d and G (not n).

Remark 2.3.6. These bounds can be expressed more symmetrically as

$$\|\mathrm{op}[p]\,\mathrm{op}[q] - \mathrm{op}[c_n]\|_1 \leqslant C_{d,G} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+4d+2}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{|\partial^{\boldsymbol{s}} F_{n+1}(\boldsymbol{x},\boldsymbol{y})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^G}\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y},$$

$$\|\mathrm{op}[p]\,\mathrm{op}[q] - \mathrm{op}[c_n]\| \leqslant C'_{d,G} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+3d+3}} \sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \int_{\{\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^{2d}:\frac{1}{2}(\boldsymbol{x}+\boldsymbol{y})=\boldsymbol{z}\}} \frac{|\partial^{\boldsymbol{s}} F_{n+1}(\boldsymbol{x},\boldsymbol{y})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^G}\, \mu_{2d}(\mathrm{d}(\boldsymbol{x},\boldsymbol{y})).$$

(The surface element $\mu_{2d}(\mathrm{d}(\boldsymbol{x},\boldsymbol{y}))$ in the second integral indicates that it is only a $2d$-dimensional integral over a subset of $(\boldsymbol{x},\boldsymbol{y})$ space.)

Proof. <u>Bound for $\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})$.</u> Change variables $\boldsymbol{x} = \boldsymbol{u} + \frac{1}{2}\boldsymbol{v}$ and $\boldsymbol{y} = \boldsymbol{u} - \frac{1}{2}\boldsymbol{v}$. This satisfies

$$\sigma(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v})_1 \cdot (\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v})_2 - (\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v})_1 \cdot (\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v})_2 = \sigma(\boldsymbol{v},\boldsymbol{u}),$$

and for each $j \in \{1,\dots,2d\}$ has Jacobian determinant

$$\det J = \det\begin{pmatrix} \frac{\partial x_j}{\partial u_j} & \frac{\partial x_j}{\partial v_j} \\ \frac{\partial y_j}{\partial u_j} & \frac{\partial y_j}{\partial v_j} \end{pmatrix} = \det\begin{pmatrix} 1 & \frac{1}{t} \\ t & -1 \end{pmatrix} = -1.$$

Then changing variables $t\boldsymbol{u}' = \sqrt{t}\,\boldsymbol{u}$ and $\boldsymbol{v}' = \sqrt{t}\,\boldsymbol{v}$ gives

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v}\big) \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t.$$

As before, we denote $\widetilde{\nabla}_{\boldsymbol{y}} := (\nabla_{\boldsymbol{y}_2}, -\nabla_{\boldsymbol{y}_1})$, so that $\widetilde{\nabla}_{\boldsymbol{x}} \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})} = -2\mathrm{i}\boldsymbol{y}\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}$. Define the operator

$$P_{\boldsymbol{x},\boldsymbol{y}} := \frac{1 + \frac{1}{2}\mathrm{i}\boldsymbol{y} \cdot \widetilde{\nabla}_{\boldsymbol{x}}}{1 + |\boldsymbol{y}|^2} \qquad \Longrightarrow P_{\boldsymbol{x},\boldsymbol{y}}^{\mathrm{T}} = \frac{1 - \frac{1}{2}\mathrm{i}\boldsymbol{y} \cdot \widetilde{\nabla}_{\boldsymbol{x}}}{1 + |\boldsymbol{y}|^2},$$

so that $P_{\boldsymbol{v},\boldsymbol{u}} \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})} = \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})}$ and $P_{\boldsymbol{u},\boldsymbol{v}}^{\mathrm{T}} \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})} = \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})}$. Thus, for $M, N \in \mathbb{N}_0$,

$$R_{n+1}(\boldsymbol{z}) = \frac{1}{\pi^{2d}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) \Big((P_{\boldsymbol{u},\boldsymbol{v}})^M (P_{\boldsymbol{v},\boldsymbol{u}}^{\mathrm{T}})^L F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v}\big)\Big) \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t.$$

Applying Lemma 2.2.4 with $\boldsymbol{a} = \boldsymbol{0}$ for $\boldsymbol{v}$ and with $|\boldsymbol{a}| \leqslant M$ for $\boldsymbol{u}$, and bounding powers of $\frac{1}{2}$ by 1, this shows that

$$\begin{aligned} &|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \\ &\quad \leqslant C_{L,M} \sum_{|\boldsymbol{l}| \leqslant L} \sum_{|\boldsymbol{m}| \leqslant M} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) \frac{\big|\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_{\boldsymbol{u}}^{\boldsymbol{m}} \partial_{\boldsymbol{v}}^{\boldsymbol{l}} F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \frac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \frac{1}{2}\boldsymbol{v}\big)\big|}{\langle \boldsymbol{u}\rangle^L \langle \boldsymbol{v}\rangle^M} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t, \end{aligned}$$

where $C_{L,M}$ is a constant.

Application of chain rule. Applying the chain rule, we find that

$$\begin{aligned} &\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_{\boldsymbol{u}}^{\boldsymbol{m}} \partial_{\boldsymbol{v}}^{\boldsymbol{l}} F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v}\big) \\ &\quad = (-t)^{|\boldsymbol{m}|} \big(\tfrac{1}{2}\big)^{|\boldsymbol{l}|} \sum_{\boldsymbol{k}' \leqslant \boldsymbol{k}} \sum_{\boldsymbol{l}' \leqslant \boldsymbol{l}} \sum_{\boldsymbol{m}' \leqslant \boldsymbol{m}} (-1)^{|\boldsymbol{l}'|} \binom{\boldsymbol{k}}{\boldsymbol{k}'} \binom{\boldsymbol{l}}{\boldsymbol{l}'} \binom{\boldsymbol{m}}{\boldsymbol{m}'} \partial_{\boldsymbol{x}}^{\boldsymbol{k}'+\boldsymbol{l}'+\boldsymbol{m}'} \partial_{\boldsymbol{y}}^{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}-(\boldsymbol{k}'+\boldsymbol{l}'+\boldsymbol{m}')} F_{n+1}(\boldsymbol{x}, \boldsymbol{y}), \end{aligned}$$

where $\boldsymbol{x}$ and $\boldsymbol{y}$ take the values $\boldsymbol{x} = \boldsymbol{z} - t\boldsymbol{u} - \frac{1}{2}\boldsymbol{v}$ and $\boldsymbol{y} = \boldsymbol{z} - t\boldsymbol{u} + \frac{1}{2}\boldsymbol{v}$. Summing over $\boldsymbol{k}$, $\boldsymbol{l}$, $\boldsymbol{m}$, taking the absolute value and applying the triangle inequality, we obtain a linear combination of absolute values of derivatives of F_{n+1}. Bounding $|t| \leqslant 1$ and $\frac{1}{2} \leqslant 1$, and bounding the combinatorial coefficients by their maximum $C_{K,L,M}$, we obtain

$$\begin{aligned} &\sum_{|\boldsymbol{k}| \leqslant K} \sum_{|\boldsymbol{l}| \leqslant L} \sum_{|\boldsymbol{m}| \leqslant M} \big|\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_{\boldsymbol{u}}^{\boldsymbol{m}} \partial_{\boldsymbol{v}}^{\boldsymbol{l}} F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v}\big)\big| \\ &\qquad \leqslant C_{K,L,M} \sum_{\substack{\boldsymbol{s} \in \mathbb{N}_0^{4d} \\ |\boldsymbol{s}| \leqslant K+L+M}} \big|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z} - t\boldsymbol{u} - \tfrac{1}{2}\boldsymbol{v}, \boldsymbol{z} - t\boldsymbol{u} + \tfrac{1}{2}\boldsymbol{v}\big)\big|. \end{aligned}$$

Thus, setting $C' := C_{L,M} C_{K,L,M}$, we have

$$\sum_{|\boldsymbol{k}|\leqslant K} |\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \leqslant C' \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant K+L+M}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-t\boldsymbol{u}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}-t\boldsymbol{u}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{u}\rangle^L \langle \boldsymbol{v}\rangle^M} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t.$$

Trace norm bound. Substituting the above into the trace norm bound of Lemma 2.1.3, with $K = 2d+1$, $L = 2d+1$, $M = G$, we find that $\|\operatorname{op}[R_{n+1}]\|_1$ is bounded by a constant multiple of

$$\sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+4d+2}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-t\boldsymbol{u}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}-t\boldsymbol{u}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{u}\rangle^{2d+1} \langle \boldsymbol{v}\rangle^G} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}t.$$

Changing variables $\boldsymbol{z}' := \boldsymbol{z} - t\boldsymbol{u}$, we find that this equals

$$\sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+4d+2}} \left(\int_0^1 g_n(t)\,\mathrm{d}t\right)\left(\int_{\mathbb{R}^{2d}} \frac{1}{\langle \boldsymbol{u}\rangle^{2d+1}}\,\mathrm{d}\boldsymbol{u}\right)\left(\int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{v}\rangle^G} \,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{z}\right).$$

Evaluating the $\mathrm{d}t$ integral (which equals 1) and the $\mathrm{d}\boldsymbol{u}$ integral gives the stated bound.

Operator norm bound. For any $q \in C_{\mathrm{b}}^\infty(\mathbb{R}^{2d})$, we may write the operator norm bound in Lemma 2.1.2 as

$$\|\operatorname{op}[q]\| \leqslant C_d \sup_{\boldsymbol{z}\in L^\infty(\mathbb{R}^{2d})} \max_{|\boldsymbol{k}|\leqslant d+2} |\partial^{\boldsymbol{k}} q(\boldsymbol{z})| \leqslant C_d \sup_{\boldsymbol{z}\in L^\infty(\mathbb{R}^{2d})} \sum_{|\boldsymbol{k}|\leqslant d+2} |\partial^{\boldsymbol{k}} q(\boldsymbol{z})|.$$

Applying this with the above bound for R_{n+1}, with $K = d+2$, $L = 2d+1$, $M = G$, we find that $\|\operatorname{op}[R_{n+1}]\|$ is bounded by a constant multiple of

$$\begin{aligned}
&\sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+3d+3}} \int_0^1 \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} g_n(t) \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-t\boldsymbol{u}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}-t\boldsymbol{u}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{u}\rangle^{2d+1} \langle \boldsymbol{v}\rangle^G} \,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t \\
&\leqslant \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+3d+3}} \int_0^1 \int_{\mathbb{R}^{2d}} \sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \left(\int_{\mathbb{R}^{2d}} g_n(t) \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-t\boldsymbol{u}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}-t\boldsymbol{u}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{u}\rangle^{2d+1} \langle \boldsymbol{v}\rangle^G} \,\mathrm{d}\boldsymbol{v}\right)\mathrm{d}\boldsymbol{u}\,\mathrm{d}t \\
&= \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d} \\ |\boldsymbol{s}|\leqslant G+3d+3}} \int_0^1 \int_{\mathbb{R}^{2d}} \sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \left(\int_{\mathbb{R}^{2d}} g_n(t) \frac{\left|\partial^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z}-\frac{1}{2}\boldsymbol{v}, \boldsymbol{z}+\frac{1}{2}\boldsymbol{v}\big)\right|}{\langle \boldsymbol{u}\rangle^{2d+1} \langle \boldsymbol{v}\rangle^G} \,\mathrm{d}\boldsymbol{v}\right)\mathrm{d}\boldsymbol{u}\,\mathrm{d}t.
\end{aligned}$$

As with the trace norm bound, we may now evaluate the $\mathrm{d}t$ and $\mathrm{d}\boldsymbol{u}$ integrals. □

Remark 2.3.7. The trace norm bound could be viewed as an analogue of the formula

$$\operatorname{tr}\big(\operatorname{op}[p]\operatorname{op}[q]\big) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} p(\boldsymbol{z}) q(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}.$$

This identity is well known (see for example Robert, 1987, Proposition (II-56)) and can be proved by following the proof of Lemma 2.3.5. Substituting $p \,\#\, q$ into the trace formula gives

$$\operatorname{tr}\big(\operatorname{op}[p]\operatorname{op}[q]\big) = \frac{1}{\pi^{2d}} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} p(\boldsymbol{z}-\boldsymbol{x}) q(\boldsymbol{z}-\boldsymbol{y}) \mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{x},\boldsymbol{y})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z},$$

then changing variables and interchanging the order of integration gives

$$\begin{aligned}\operatorname{tr}\big(\mathrm{op}[p]\,\mathrm{op}[q]\big) &= \frac{1}{\pi^{2d}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} p(\boldsymbol{z}-(\boldsymbol{u}+\tfrac{1}{2}\boldsymbol{v}))q(\boldsymbol{z}-(\boldsymbol{u}-\tfrac{1}{2}\boldsymbol{v}))\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})}\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\\ &= \frac{1}{\pi^{2d}}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} p(\boldsymbol{z}-\tfrac{1}{2}\boldsymbol{v})q(\boldsymbol{z}+\tfrac{1}{2}\boldsymbol{v})\,\mathrm{e}^{2\mathrm{i}\sigma(\boldsymbol{v},\boldsymbol{u})}\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v},\end{aligned}$$

and then the formula follows from the Fourier inversion theorem.

Remark 2.3.8. The proof of Lemma 2.3.5 begins with the interesting observation that the change of variables from $\boldsymbol{x},\boldsymbol{y}$ to $\boldsymbol{u},\boldsymbol{v}$ preserves the symplectic form σ. This perhaps gives the false impression that this is critical to proving the result, when in fact it just allows the bounds to be slightly neater than they otherwise would be. We could have proceeded with the start of the proof in precisely the same way without this change of variables, giving the bound

$$|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \leqslant C_{S,T}\sum_{|\boldsymbol{s}|\leqslant S}\sum_{|\boldsymbol{t}|\leqslant T}\int_0^1\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} g_n(t)\frac{\big|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}\partial_{\boldsymbol{x}}^{\boldsymbol{t}}\partial_{\boldsymbol{y}}^{\boldsymbol{s}}F_{n+1}\big(\boldsymbol{z}-\sqrt{t}\boldsymbol{x},\boldsymbol{z}-\sqrt{t}\boldsymbol{y}\big)\big|}{\langle\boldsymbol{x}\rangle^S\langle\boldsymbol{y}\rangle^T}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}t,$$

where again $g_n(t) := (n+1)(1-t)^n$. We could have changed variables $\boldsymbol{x}=\boldsymbol{u}+\frac{1}{2}\boldsymbol{v}$, $\boldsymbol{y}=\boldsymbol{u}-\frac{1}{2}\boldsymbol{v}$ at this later point, putting $S=T=G+2d+1$ and using Lemma 2.2.2 to bound the denominator. Working in exactly the same way as in the rest of the proof, this gives the bounds

$$\begin{aligned}\|\mathrm{op}[R_{n+1}]\|_1 &\leqslant C_{d,G}\sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d}\\|\boldsymbol{s}|\leqslant 2G+6d+3}}\int_0^1\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} g_n(t)\frac{\big|\partial^{\boldsymbol{s}}F_{n+1}\big(\boldsymbol{z}-\frac{1}{2}\sqrt{t}\boldsymbol{v},\boldsymbol{z}+\frac{1}{2}\sqrt{t}\boldsymbol{v}\big)\big|}{\langle\boldsymbol{v}\rangle^G}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{z}\,\mathrm{d}t,\\ \|\mathrm{op}[R_{n+1}]\| &\leqslant C'_{d,G}\sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d}\\|\boldsymbol{s}|\leqslant 2G+5d+4}}\sup_{\boldsymbol{z}\in\mathbb{R}^{2d}}\int_0^1\int_{\mathbb{R}^{2d}} g_n(t)\frac{\big|\partial^{\boldsymbol{s}}F_{n+1}\big(\boldsymbol{z}-\frac{1}{2}\sqrt{t}\boldsymbol{v},\boldsymbol{z}+\frac{1}{2}\sqrt{t}\boldsymbol{v}\big)\big|}{\langle\boldsymbol{v}\rangle^G}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}t.\end{aligned}$$

The presence of the integral in t would be an inconvenience, but nothing more.

To use Lemma 2.3.5 in this thesis, the requirement that p and q be Schwartz is too strict. In the next lemma we show that this condition can be relaxed.

Lemma 2.3.9. *Let $p,q\in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ and $n,G\in\mathbb{N}_0$ such that $G>2d$ and p (or q) satisfies*

$$\partial^{\boldsymbol{m}}p\in L^1(\mathbb{R}^{2d}),\quad \textit{for all } \boldsymbol{m}\in\mathbb{N}_0^{2d}.$$

Then the trace norm inequality in Lemma 2.3.5 holds, with the same constant $C_{d,G}$.

Proof. Notation. Let $A := \mathrm{op}[p]\,\mathrm{op}[q]-\mathrm{op}[c_n]$ and let

$$I := C_{d,G}\sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d}\\|\boldsymbol{s}|\leqslant G+4d+2}}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\frac{|\partial^{\boldsymbol{s}}F_{n+1}(\boldsymbol{x},\boldsymbol{y})|}{\langle\boldsymbol{x}-\boldsymbol{y}\rangle^G}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}.$$

We must show that $\|A\|_1\leqslant I$. Let ζ be a smooth function on $\mathbb{R}^{2d}$ satisfying

$$\zeta(\boldsymbol{z}) = \begin{cases}1 & \text{when } |\boldsymbol{z}|\leqslant 1,\\ 0 & \text{when } |\boldsymbol{z}|\geqslant 2.\end{cases}$$

For each $N\in\mathbb{N}$ (where $\mathbb{N}$ is the set of strictly positive natural numbers) we define $p_{(N)}(\boldsymbol{z}):=\zeta(\boldsymbol{z}/N)p(\boldsymbol{z})$, and $q_{(N)}$ similarly, and we define $c_{n;(N)}$, $F_{n+1;(N)}$, $A_{(N)}$ and $I_{(N)}$ in terms of $p_{(N)}$ and $q_{(N)}$ just as c_n, F_{n+1}, A and I are defined in terms of p and q. For each $M,N\in\mathbb{N}$ such that $N\geqslant M$ we define $p_{(M,N)}(\boldsymbol{z}):=\big(\zeta(\boldsymbol{z}/N)-\zeta(\boldsymbol{z}/M)\big)p(\boldsymbol{z})$, and define $q_{(M,N)}$, $c_{n;(M,N)}$ and $F_{n+1;(M,N)}$ as before.

Boundedness of symbols. We will need the simple observation that $p_{(N)}$, $q_{(N)}$, $c_{n;(N)}$ and $F_{n+1;(N)}$ and their derivatives are all bounded, with bounds that do not depend on N. To see this, first note that for any multi-index $\boldsymbol{a}\in\mathbb{N}_0^{2d}$ we have

$$\partial_{\boldsymbol{z}}^{\boldsymbol{a}}(p_{(N)}(\boldsymbol{z}))=\sum_{\boldsymbol{b}\leqslant\boldsymbol{a}}\binom{\boldsymbol{a}}{\boldsymbol{b}}(\partial_{\boldsymbol{z}}^{\boldsymbol{b}}p(\boldsymbol{z}))(\partial_{\boldsymbol{z}}^{\boldsymbol{a}-\boldsymbol{b}}\zeta(\boldsymbol{z}/N))=\sum_{\boldsymbol{b}\leqslant\boldsymbol{a}}\binom{\boldsymbol{a}}{\boldsymbol{b}}\frac{1}{N^{\boldsymbol{a}-\boldsymbol{b}}}(\partial^{\boldsymbol{b}}p(\boldsymbol{z}))(\partial^{\boldsymbol{a}-\boldsymbol{b}}\zeta(\boldsymbol{z}/N)).$$

Thus, for each $\boldsymbol{z}\in\mathbb{R}^{2d}$, we have

$$|\partial_{\boldsymbol{z}}^{\boldsymbol{a}}(p_{(N)}(\boldsymbol{z}))|\leqslant\sum_{\boldsymbol{b}\leqslant\boldsymbol{a}}\binom{\boldsymbol{a}}{\boldsymbol{b}}|\partial^{\boldsymbol{b}}p(\boldsymbol{z})\partial^{\boldsymbol{a}-\boldsymbol{b}}\zeta(\boldsymbol{z}/N)|\leqslant 2^{|\boldsymbol{a}|}\Big(\sup_{\boldsymbol{u}\in\mathbb{R}^{2d}}\max_{\boldsymbol{b}\leqslant\boldsymbol{a}}|\partial^{\boldsymbol{b}}\zeta(\boldsymbol{u})|\Big)\Big(\max_{\boldsymbol{b}\leqslant\boldsymbol{a}}|\partial^{\boldsymbol{b}}p(\boldsymbol{z})|\Big).$$

Combined with the fact that $p\in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$, this proves that $p_{(N)}$ and its derivatives are bounded uniformly on $N\in\mathbb{N}$. The same is true of $q_{(N)}$ for the same reason. To show the analogous inequality for $c_{n;(N)}$, apply the observation in Remark 2.3.4, which implies that

$$|\partial^{\boldsymbol{a}}c_{n;(N)}(\boldsymbol{z})|\leqslant\sum_{|\boldsymbol{m}|\leqslant n}\frac{1}{|\boldsymbol{m}|!2^{|\boldsymbol{m}|}}\left|\partial_{\boldsymbol{z}}^{\boldsymbol{a}}\big(\partial^{\boldsymbol{m}}p_{(N)}(\boldsymbol{z})\partial^{\tau(\boldsymbol{m})}q_{(N)}(\boldsymbol{z})\big)\right|,$$

then apply the product rule for $\partial_{\boldsymbol{z}}^{\boldsymbol{a}}$ and use the above bounds for derivatives of $p_{(N)}$ and $q_{(N)}$. Similarly, we have

$$|\partial_{\boldsymbol{x}}^{\boldsymbol{a}}\partial_{\boldsymbol{y}}^{\boldsymbol{b}}F_{n+1;(N)}(\boldsymbol{x},\boldsymbol{y})|\leqslant\sum_{|\boldsymbol{m}|=n+1}\frac{1}{|\boldsymbol{m}|!2^{|\boldsymbol{m}|}}\left|\partial^{\boldsymbol{a}+\boldsymbol{m}}p_{(N)}(\boldsymbol{x})\partial^{\boldsymbol{b}+\tau(\boldsymbol{m})}q_{(N)}(\boldsymbol{y})\right|,$$

and using the above bounds for $p_{(N)}$ and $q_{(N)}$ gives a bound for $F_{n+1;(N)}$.

$A_{(N)}\to A$ weakly. It suffices to consider $u,v\in\mathscr{S}(\mathbb{R}^d)$ because $\mathscr{S}(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$. We have

$$\langle A_{(N)}u,v\rangle-\langle Au,v\rangle=\langle(\mathrm{op}[p_{(N)}]\,\mathrm{op}[q_{(N)}]-\mathrm{op}[p]\,\mathrm{op}[q])u,v\rangle+\langle(\mathrm{op}[c_{n;(N)}]-\mathrm{op}[c_n])u,v\rangle.$$

First we will show that $\mathrm{op}[c_{n;(N)}]\to\mathrm{op}[c_n]$ weakly. We have

$$\langle(\mathrm{op}[c_{n;(N)}]-\mathrm{op}[c_n])u,v\rangle=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi}(c_{n;(N)}-c_n)\big(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}),\xi\big)u(\boldsymbol{y})\overline{v(\boldsymbol{x})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\xi\,\mathrm{d}\boldsymbol{x},$$

Integrating by parts with the operator defined in Notation 2.2.3, we find that this equals

$$\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi}(P_{\boldsymbol{y},\xi}^{\mathrm{T}})^{d+1}\Big((c_{n;(N)}-c_n)\big(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}),\xi\big)u(\boldsymbol{y})\Big)\overline{v(\boldsymbol{x})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\xi\,\mathrm{d}\boldsymbol{x}.$$

We bound the absolute value of this integral. For $\left|\big(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}),\xi\big)\right|\leqslant N$, this integrand is zero. Elsewhere, we bound c_n and its derivatives by their suprema, and bound $c_{n;(N)}$ as shown above, which gives a bound that does not depend on N. We use Lemma 2.2.4 to obtain decay in ξ, and the fact that u (and its derivatives) and v are Schwartz to obtain decay in $\boldsymbol{y}$ and $\boldsymbol{x}$ respectively. This implies that

$$|\langle(\mathrm{op}[c_{n;(N)}]-\mathrm{op}[c_n])u, v\rangle| \leqslant C \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{\chi_{[N,\infty)}\left(\left|\left(\frac{1}{2}(\boldsymbol{x}+\boldsymbol{y}), \xi\right)\right|\right)}{\langle\xi\rangle^{d+1}\langle\boldsymbol{x}\rangle^{d+1}\langle\boldsymbol{y}\rangle^{d+1}}\, \mathrm{d}\boldsymbol{y}\, \mathrm{d}\xi\, \mathrm{d}\boldsymbol{x},$$

where C depends on u, v, p and q (and our choice of ζ) but not $\boldsymbol{y}$, ξ, $\boldsymbol{x}$ or N. We may now apply Lebesgue's dominated convergence theorem on this integral, and since the pointwise limit of the integrand is zero this implies that the overall limit is zero as $N \to \infty$. This completes the proof of the claim that $\mathrm{op}[c_{n;(N)}] \to \mathrm{op}[c_n]$ weakly.

Now we will show that $\mathrm{op}[p_{(N)}]\mathrm{op}[q_{(N)}] \to \mathrm{op}[p]\mathrm{op}[q]$ weakly. We have

$$\begin{aligned}&\langle(\mathrm{op}[p]\mathrm{op}[q]-\mathrm{op}[p_{(N)}]\mathrm{op}[q_{(N)}])u, v\rangle\\ &\qquad = \langle(\mathrm{op}[p]\mathrm{op}[q]-\mathrm{op}[p]\mathrm{op}[q_{(N)}])u, v\rangle + \langle(\mathrm{op}[p]\mathrm{op}[q_{(N)}]-\mathrm{op}[p_{(N)}]\mathrm{op}[q_{(N)}])u, v\rangle.\end{aligned}$$

But setting $\tilde{v} := \mathrm{op}[\overline{p}]v \in \mathscr{S}(\mathbb{R}^{2d})$ we have

$$\langle(\mathrm{op}[p]\mathrm{op}[q]-\mathrm{op}[p]\mathrm{op}[q_{(N)}])u, v\rangle = \langle(\mathrm{op}[q]-\mathrm{op}[q_{(N)}])u, \tilde{v}\rangle,$$

and setting $\tilde{u} := \mathrm{op}[q_{(N)}]u \in \mathscr{S}(\mathbb{R}^{2d})$ we have

$$\langle(\mathrm{op}[p]\mathrm{op}[q_{(N)}]-\mathrm{op}[p_{(N)}]\mathrm{op}[q_{(N)}])u, v\rangle = \langle(\mathrm{op}[p]-\mathrm{op}[p_{(N)}])\tilde{u}, v\rangle,$$

and by the same reasoning as $c_{n,N}$ these both also converge to zero. Thus $A_N \to A$ weakly.

<u>$A_{(N)} \to A$ in trace norm.</u> We will first show that $A_{(N)}$ is a Cauchy sequence in trace norm. For each $M, N \in \mathbb{N}$ with $N \geqslant M$ we have $p_{(M,N)}, q_{(M,N)} \in \mathscr{S}(\mathbb{R}^{2d})$, so we may apply Lemma 2.3.5 (with $G = 2d+1$) giving

$$\|A_{(N)} - A_{(M)}\|_1 \leqslant C_{d,2d+1} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d}\\ |\boldsymbol{s}|\leqslant 6d+3}} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{|\partial^{\boldsymbol{s}} F_{n+1;(M,N)}(\boldsymbol{x},\boldsymbol{y})|}{\langle\boldsymbol{x}-\boldsymbol{y}\rangle^{2d+1}}\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y}.$$

But we may bound $F_{n+1;(M,N)}$ in the same way that we bounded $F_{n+1;(N)}$, using the triangle inequality to bound derivatives of $\zeta(\boldsymbol{z}/N) - \zeta(\boldsymbol{z}/M)$ in terms of derivatives of ζ, and also bounding q and its derivatives by their suprema; this gives

$$\|A_{(N)} - A_{(M)}\|_1 \leqslant K \sum_{|\boldsymbol{m}|\leqslant 6d+3+n+1} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{\chi_{[M,\infty)}(|(\boldsymbol{x},\boldsymbol{y})|)|\partial^{\boldsymbol{m}} p(\boldsymbol{x})|}{\langle\boldsymbol{x}-\boldsymbol{y}\rangle^{2d+1}}\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y}$$

for some value K that does not depend on M or N. As before, an application of Lebesgue's dominated convergence theorem shows that the limit of this expression is zero as $M, N \to \infty$. Thus $A_{(N)}$ is a Cauchy sequence in the trace norm topology, and since the space of trace class operators is complete (Birman and Solomjak, 1987, Theorem 11.2.6), this sequence is trace norm convergent, and its limit matches the weak limit so $A_{(N)} \to A$ in trace norm.

<u>$I_{(N)} \to I$.</u> For $|(\boldsymbol{x},\boldsymbol{y})| \leqslant N$ we have $F_{n+1}(\boldsymbol{x},\boldsymbol{y}) = F_{n+1;(N)}(\boldsymbol{x},\boldsymbol{y})$, so (using the fact that $G > 2d$)

$$\begin{aligned}|I_{(N)} - I| &\leqslant C_{d,G} \sum_{\substack{\boldsymbol{s}\in\mathbb{N}_0^{4d}\\ |\boldsymbol{s}|\leqslant G+4d+2}} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{\chi_{[N,\infty)}(|(\boldsymbol{x},\boldsymbol{y})|)\big(|\partial^{\boldsymbol{s}} F_{n+1;(N)}(\boldsymbol{x},\boldsymbol{y})| + |\partial^{\boldsymbol{s}} F_{n+1}(\boldsymbol{x},\boldsymbol{y})|\big)}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^{G}}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\\ &\leqslant K' \sum_{|\boldsymbol{m}|\leqslant G+4d+2+n+1} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{\chi_{[N,\infty)}(|(\boldsymbol{x},\boldsymbol{y})|)|\partial^{\boldsymbol{m}} p(\boldsymbol{x})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^{2d+1}}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}.\end{aligned}$$

Again using Lebesgue's dominated convergence theorem, we see that the limit of this is zero as $N \to \infty$.

<u>Conclusion.</u> For each $N \in \mathbb{N}$ we have $p_{(N)}, q_{(N)} \in \mathscr{S}(\mathbb{R}^{2d})$, so we may apply Lemma 2.3.5, giving $\|A_{(N)}\|_1 \leqslant I_{(N)}$. We have shown that $I_{(N)} \to I$ as $N \to \infty$, and we also have

$$\Big| \|A_{(N)}\|_1 - \|A\|_1 \Big| \leqslant \|A_{(N)} - A\|_1 \to 0,$$

so $\|A_{(N)}\|_1 \to \|A\|_1$ as $N \to \infty$. Thus $\|A\|_1 \leqslant I$, which is what we were required to prove. □

Remark 2.3.10. It may appear at first glance that a trivial modification of the above proof allows us to drop the assumption that $\partial^{\boldsymbol{m}} p \in L^1(\mathbb{R}^{2d})$, instead using the fact that I is finite (because if not the conclusion of the lemma is vacuous). The apparent modification is to bound $\|A_{(N)} - A_{(M)}\|_1$ and $|I_{(N)} - I|$ in terms of $|\partial^{\boldsymbol{m}} F_{n+1}(\boldsymbol{x},\boldsymbol{y})|$ instead of $|\partial^{\boldsymbol{m}} p(\boldsymbol{x})|$. However, $F_{n+1;(N)}$ is defined in terms of $p_{(N)}$ and $q_{(N)}$ rather than simply being F_{n+1} multiplied by $\zeta(\boldsymbol{x}/N)\zeta(\boldsymbol{y}/N)$, which is why the first bound for it (under "boundedness of symbols") was not simply in terms of F_{n+1} and ζ. Put another way, there may be cancellation between the terms making up F_{n+1} so that even when it is small the individual terms may be large.

2.4 Comparison with usual remainder bounds

As discussed at the very start of this chapter, the composition of two pseudodifferential operators is often expressed as an asymptotic series, with the truncation to a finite series guaranteed to be "small" in some sense. This bound usually just relies on the fact that the remainder involves increasing numbers of derivatives as more terms are included in the finite series; such a proof starts by essentially showing Lemma 2.3.3, and then uses rough bounds to throw away a lot of information. In this section we prove such a rough bound, Lemma 2.4.2, and illustrate how it can be used to show that the remainder is in the required symbol class and has the required semiclassical asymptotics. In §5.7 we will consider why the corresponding trace norm bound is not sufficient for the main result of this thesis, which explains why we need the more delicate bound derived at the end of §2.3.

Notation 2.4.1. For any $p \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ and $\boldsymbol{z} \in \mathbb{R}^{2d}$, denote

$$[p]_{L,M}(\boldsymbol{z}) := \max_{L\leqslant|\boldsymbol{k}|\leqslant L+M} |\partial^{\boldsymbol{k}} p(\boldsymbol{z})|.$$

Lemma 2.4.2. *For any $p, q \in \mathscr{S}(\mathbb{R}^{2d})$ and $n \in \mathbb{N}_0$, define R_{n+1} as in Lemma 2.3.3. Let $\boldsymbol{k} \in \mathbb{N}_0^{2d}$. Then*

$$|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \leqslant C \sum_{l=0}^{|\boldsymbol{k}|} \int_0^1 \left(\int_{\mathbb{R}^{2d}} \frac{[p]_{n+1+l,T}(\boldsymbol{z} - \sqrt{t}\boldsymbol{x})}{\langle \boldsymbol{x} \rangle^S} \, \mathrm{d}\boldsymbol{x} \right) \left(\int_{\mathbb{R}^{2d}} \frac{[q]_{n+1+|\boldsymbol{k}|-l,S}(\boldsymbol{z} - \sqrt{t}\boldsymbol{y})}{\langle \boldsymbol{y} \rangle^T} \, \mathrm{d}\boldsymbol{y} \right) \mathrm{d}t,$$

where C is a constant depending on $\boldsymbol{k}, n, S, T$ (but not p or q).

Proof. Using the expression for F_{n+1} in Remark 2.3.4, we find that

$$\begin{aligned}
&\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_{\boldsymbol{x}}^{\boldsymbol{t}} \partial_{\boldsymbol{y}}^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z} - \sqrt{t}\boldsymbol{x}, \boldsymbol{z} - \sqrt{t}\boldsymbol{y}\big) \\
&\quad = (-\sqrt{t})^{|\boldsymbol{s}|+|\boldsymbol{t}|} \sum_{\boldsymbol{l} \leqslant \boldsymbol{k}} \binom{\boldsymbol{k}}{\boldsymbol{l}} \partial_{\boldsymbol{p}}^{\boldsymbol{t}+\boldsymbol{l}} \partial_{\boldsymbol{q}}^{\boldsymbol{s}+\boldsymbol{k}-\boldsymbol{l}} F_{n+1}(\boldsymbol{p}, \boldsymbol{q}) \Big|_{\substack{\boldsymbol{p} = \boldsymbol{z} - \sqrt{t}\boldsymbol{x} \\ \boldsymbol{q} = \boldsymbol{z} - \sqrt{t}\boldsymbol{y}}} \\
&\quad = (-\sqrt{t})^{|\boldsymbol{s}|+|\boldsymbol{t}|} \sum_{\boldsymbol{l} \leqslant \boldsymbol{k}} \sum_{|\boldsymbol{m}|=n+1} \binom{\boldsymbol{k}}{\boldsymbol{l}} \frac{\mathrm{i}^{n+1}}{(n+1)! 2^{n+1}} (-1)^{|\boldsymbol{m}_2|} \partial^{\boldsymbol{m}+\boldsymbol{l}+\boldsymbol{t}} p(\boldsymbol{z} - \sqrt{t}\boldsymbol{x}) \partial^{\tau(\boldsymbol{m})+\boldsymbol{k}-\boldsymbol{l}+\boldsymbol{s}} q(\boldsymbol{z} - \sqrt{t}\boldsymbol{y}),
\end{aligned}$$

so, bounding the coefficients by their maximum and bounding $\sqrt{t} \leqslant 1$,

$$\left| \partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_{\boldsymbol{x}}^{\boldsymbol{t}} \partial_{\boldsymbol{y}}^{\boldsymbol{s}} F_{n+1}\big(\boldsymbol{z} - \sqrt{t}\boldsymbol{x}, \boldsymbol{z} - \sqrt{t}\boldsymbol{y}\big) \right| \leqslant C_{\boldsymbol{k},n,S,T} \sum_{l=0}^{|\boldsymbol{k}|} [p]_{n+1+l+|\boldsymbol{t}|,0}(\boldsymbol{z} - \sqrt{t}\boldsymbol{x}) [q]_{n+1+|\boldsymbol{k}|-l+|\boldsymbol{s}|,0}(\boldsymbol{z} - \sqrt{t}\boldsymbol{y}).$$

Substituting this into the bound noted in Remark 2.3.8 gives the stated result. □

Our first example of applying Lemma 2.4.2 is for symbol classes. There are many ways of classifying symbols of pseudodifferential operators, but we will focus on the Shubin classes. We could just as well have considered the Hörmander classes, but these involve the decay of the symbol $p(\boldsymbol{z})$ in terms of $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$ separately, so this would have required that we develop bounds for R_{n+1} that distinguish between these. The Shubin classes are defined as follows (Shubin, 2001, Definition 23.1).

Notation 2.4.3. Let $m \in \mathbb{R}$ and $0 < \rho \leqslant 1$. We define the symbol class $\Gamma_\rho^m(\mathbb{R}^{2d})$ as the set of every infinitely differentiable function a on $\mathbb{R}^{2d}$ for which, for each $\boldsymbol{k} \in \mathbb{N}_0^{2d}$, there exists a constant $C_{\boldsymbol{k}}$ such that

$$|\partial^{\boldsymbol{k}} a(\boldsymbol{z})| \leqslant C_{\boldsymbol{k}} \langle \boldsymbol{z} \rangle^{m - \rho|\boldsymbol{k}|}, \qquad \text{for all } \boldsymbol{z} \in \mathbb{R}^{2d}.$$

Theorem 2.4.4 (Shubin, 2001, Theorem 23.6)**.** *For $p \in \Gamma_\rho^{m_1}$, $q \in \Gamma_\rho^{m_2}$ we have*

$$p \# q(\boldsymbol{z}) = \sum_{j=0}^{n} F_j(\boldsymbol{z}, \boldsymbol{z}) + R_{n+1}(\boldsymbol{z})$$

where $F_j(\boldsymbol{z}, \boldsymbol{z}) \in \Gamma_\rho^{m_1+m_2-2\rho j}$ and $R_{n+1} \in \Gamma_\rho^{m_1+m_2-2\rho(n+1)}$.

Remark 2.4.5. A complete proof of Theorem 2.4.4 for general p, q would require discussion of oscillatory integrals, which will not be needed elsewhere in this thesis and would not help illuminate the comparison with other remainder bounds; therefore we will prove this result only for $p, q \in \mathscr{S}(\mathbb{R}^{2d})$. The literal interpretation of this result is trivial in this case, because as proved in

Remark 2.3.4 this immediately implies that $F_j(\boldsymbol{z},\boldsymbol{z}) \in \mathscr{S}(\mathbb{R}^{2d})$ and $R_{n+1} \in \mathscr{S}(\mathbb{R}^{2d})$, so they are in all the Shubin classes. However, the essential idea of Theorem 2.4.4 is that each $\Gamma_\rho^{m_1+m_2-2\rho(n+1)}$ semi-norm of R_{n+1} is bounded in terms of a finite number of $\Gamma_\rho^{m_1}$ semi-norms of p and $\Gamma_\rho^{m_2}$ semi-norms of q; that is,

$$|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \leqslant C_{\boldsymbol{k}} \langle \boldsymbol{z} \rangle^{m_1+m_2-2\rho(n+1)-\rho|\boldsymbol{k}|},$$

where $C_{\boldsymbol{k}}$ depends on p and q only via a finite number of their constants in the defining condition of $\Gamma_\rho^{m_1}$ and $\Gamma_\rho^{m_2}$. This is non-trivial even when $p, q \in \mathscr{S}(\mathbb{R}^{2d})$.

Idea of proof for Theorem 2.4.4. Summary. We prove the symbol class for R_{n+1}; the symbol class for $F_n(\boldsymbol{z},\boldsymbol{z})$ follows similarly with an analogous form of Lemma 2.4.2. We will show that the integral of $[p]_{n+1+l,T}$ is bounded by a multiple of $\langle \boldsymbol{z} \rangle^{m_1-\rho(n+1+l)}$, and similarly the integral of $[q]_{n+1+|\boldsymbol{k}|-l,S}$ is bounded by a multiple of $\langle \boldsymbol{z} \rangle^{m_1-\rho(n+1+|\boldsymbol{k}|-l)}$, which proves the result.

Integral of $[p]_{n+1+l,T}$. For each $\boldsymbol{r} \in \mathbb{N}_0^{2d}$, denote by $C_{\boldsymbol{r}}$ the constant in the defining condition for $p \in \Gamma_\rho^{m_1}$, and denote by $C'_{\boldsymbol{r}}$ the constant for $q \in \Gamma_\rho^{m_2}$. For any $L, M \in \mathbb{N}_0$ we have

$$[p]_{L,M}(\boldsymbol{z}) \leqslant \max_{L \leqslant |\boldsymbol{r}| \leqslant L+M} \Big(C_{\boldsymbol{r}} \langle \boldsymbol{z} \rangle^{m_1-\rho|\boldsymbol{r}|} \Big) \leqslant \langle \boldsymbol{z} \rangle^{m_1-\rho L} \max_{L \leqslant |\boldsymbol{r}| \leqslant L+M} C_{\boldsymbol{r}},$$

so for any $l \in \mathbb{N}_0$ we have

$$\int_{\mathbb{R}^{2d}} \frac{[p]_{n+1+l,T}(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})}{\langle \boldsymbol{x} \rangle^S} \,\mathrm{d}\boldsymbol{x} \leqslant \Big(\max_{n+1+l \leqslant |\boldsymbol{r}| \leqslant n+1+l+T} C_{\boldsymbol{r}} \Big) \int_{\mathbb{R}^{2d}} \frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^{m_1-\rho(n+1+l)}}{\langle \boldsymbol{x} \rangle^S} \,\mathrm{d}\boldsymbol{x}.$$

But Lemma 2.2.2 implies that for any $P \geqslant 0$ we have

$$\frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^P}{\langle \boldsymbol{x} \rangle^P} \leqslant \frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^P}{\langle \sqrt{t}\boldsymbol{x} \rangle^P} \leqslant (\sqrt{2})^P \langle \boldsymbol{z} \rangle^P$$

and for any $P < 0$ we have

$$\frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^P}{\langle \boldsymbol{x} \rangle^{-P}} \leqslant \frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^P}{\langle \sqrt{t}\boldsymbol{x} \rangle^{-P}} = \frac{1}{\langle \sqrt{t}\boldsymbol{x} \rangle^{-P} \langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^{-P}} \leqslant (\sqrt{2})^{-P} \frac{1}{\langle \boldsymbol{z} \rangle^{-P}} = (\sqrt{2})^{-P} \langle \boldsymbol{z} \rangle^P.$$

Let ceil denote the ceiling function i.e. ceil(x) is the least integer that is greater than or equal to x. For $l \leqslant |\boldsymbol{k}|$, applying the last three inequalities with $P = m_1 - \rho(n+1+l)$ and

$$S = \mathrm{ceil}(2d+1+|m_1-\rho(n+1)|+\rho|\boldsymbol{k}|),$$

so that $2d+1+|P| \leqslant S$, we obtain

$$\begin{aligned} &\int_{\mathbb{R}^{2d}} \frac{[p]_{n+1+l,T}(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})}{\langle \boldsymbol{x} \rangle^S} \,\mathrm{d}\boldsymbol{x} \\ &\quad \leqslant \Big(\max_{n+1 \leqslant |\boldsymbol{r}| \leqslant n+1+|\boldsymbol{k}|+T} C_{\boldsymbol{r}} \Big) \int_{\mathbb{R}^{2d}} \frac{\langle \boldsymbol{z}-\sqrt{t}\boldsymbol{x} \rangle^{m_1-\rho(n+1+l)}}{\langle \boldsymbol{x} \rangle^{2d+1} \langle \boldsymbol{x} \rangle^{m_1-\rho(n+1+l)}} \,\mathrm{d}\boldsymbol{x} \\ &\quad \leqslant (\sqrt{2})^{|m_1-\rho(n+1)|+\rho|\boldsymbol{k}|} \Big(\max_{n+1 \leqslant |\boldsymbol{r}| \leqslant n+1+|\boldsymbol{k}|+T} C_{\boldsymbol{r}} \Big) \langle \boldsymbol{z} \rangle^{m_1-\rho(n+1+l)} \int_{\mathbb{R}^{2d}} \frac{1}{\langle \boldsymbol{x} \rangle^{2d+1}} \,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

Conclusion. Choosing T similarly (with m_1 replaced by m_2) and bounding the $\mathrm{d}\boldsymbol{y}$ integral in the same way, and using these bounds in Lemma 2.4.2, we find that

$$\begin{aligned}
&|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z})| \\
&\quad\leqslant C' \sum_{l=0}^{|\boldsymbol{k}|} \Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+|\boldsymbol{k}|+T} C_{\boldsymbol{r}} \Big) \langle \boldsymbol{z} \rangle^{m_1-\rho(n+1+l)} \Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+|\boldsymbol{k}|+S} C'_{\boldsymbol{r}} \Big) \langle \boldsymbol{z} \rangle^{m_2-\rho(n+1+|\boldsymbol{k}|-l)} \\
&\quad= C'|\boldsymbol{k}| \Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+|\boldsymbol{k}|+T} C_{\boldsymbol{r}} \Big) \Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+|\boldsymbol{k}|+S} C'_{\boldsymbol{r}} \Big) \langle \boldsymbol{z} \rangle^{m_1+m_2-2\rho(n+1)-\rho|\boldsymbol{k}|},
\end{aligned}$$

where (denoting the constant from Lemma 2.4.2 by $C_{\boldsymbol{k},n,S,T}$)

$$C' = C_{\boldsymbol{k},n,S,T} (\sqrt{2})^{|m_1-\rho(n+1)|+|m_1-\rho(n+1)|+2\rho|\boldsymbol{k}|} \left(\int_{\mathbb{R}^{2d}} \frac{1}{\langle \boldsymbol{u} \rangle^{2d+1}} \,\mathrm{d}\boldsymbol{u} \right)^2. \qquad \square$$

We now prove a semiclassical composition result. This involves asymptotic sums of the form

$$A(h) = \mathrm{op}_h^{\mathrm{W}}[a_0] + h\,\mathrm{op}_h^{\mathrm{W}}[a_1] + h^2\,\mathrm{op}_h^{\mathrm{W}}[a_2] + \cdots.$$

A meaning is assigned to this asymptotic sum by defining the semiclassical operators $\mathrm{op}_h^{\mathrm{W}}[a_j]$ and specifying the requirements on the remainder when the sum is truncated to a finite number of terms. The precise definition used for the remainder varies between authors, but it always requires, roughly speaking, that it equals $h^{n+1}\,\mathrm{op}_h^{\mathrm{W}}[r(h)]$, where in some sense $r(h)$ is bounded as $h \to 0$. We will follow the convention of Dimassi and Sjöstrand (1999, Definition 7.4 and following remarks), which requires that $r(h)$ and its derivatives be bounded by an order function of the type specified below for all sufficiently small h. In contrast, Robert (1987, Définition (II-11)) also allows terms and the remainder to have additional decay in the style of Shubin classes; we have already shown how this can be treated when considering symbol classes so we will not do so again now.

Definition 2.4.6 (Dimassi and Sjöstrand, 1999, Definition 7.4)**.** We say that $m\colon \mathbb{R}^{2d} \to [0,\infty)$ is an *order function* if it is not identically equal to zero and there exist constants $C_0 > 0$ and $N > 0$ such that for all $\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^{2d}$ we have

$$m(\boldsymbol{x}) \leqslant C_0 \langle \boldsymbol{x}-\boldsymbol{y} \rangle^N m(\boldsymbol{y}).$$

Example 2.4.7. If $r \in \mathbb{R}$ and $m(\boldsymbol{x}) = \langle \boldsymbol{x} \rangle^r$, then $m(\boldsymbol{x})$ is an order function. To see this for $r \geqslant 0$, for any $\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^{2d}$ apply Lemma 2.2.2 (with $\boldsymbol{x}' = \boldsymbol{x}-\boldsymbol{y}$ and $\boldsymbol{y}' = \boldsymbol{y}$) to obtain

$$m(\boldsymbol{x}) = \langle \boldsymbol{x} \rangle^r \leqslant \left(\sqrt{2}\langle \boldsymbol{x}-\boldsymbol{y} \rangle \langle \boldsymbol{y} \rangle\right)^r = 2^{r/2} \langle \boldsymbol{x}-\boldsymbol{y} \rangle^r m(\boldsymbol{y}).$$

To see it for $r < 0$, for any $\boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^{2d}$ apply Lemma 2.2.2 (with $\boldsymbol{x}' = \boldsymbol{y}-\boldsymbol{x}$ and $\boldsymbol{y}' = \boldsymbol{x}$) to obtain

$$m(\boldsymbol{x}) = \left(\frac{1}{\langle \boldsymbol{x} \rangle}\right)^{-r} \leqslant \left(\sqrt{2}\frac{\langle \boldsymbol{y}-\boldsymbol{x} \rangle}{\langle \boldsymbol{y} \rangle}\right)^{-r} = 2^{-r/2} \langle \boldsymbol{x}-\boldsymbol{y} \rangle^{-r} m(\boldsymbol{y}).$$

Definition 2.4.8 (Dimassi and Sjöstrand, 1999, Definition 7.5)**.** Let m be an order function. Then we define $S(m)$ to be the set containing every $p \in C^\infty(\mathbb{R}^{2d})$ that, for each $\boldsymbol{k} \in \mathbb{N}_0^{2d}$, has a constant $C_{\boldsymbol{k}}$ satisfying

$$|\partial^{\boldsymbol{k}} p(\boldsymbol{z})| \leqslant C_{\boldsymbol{k}} m(\boldsymbol{z}) \qquad \text{for all } \boldsymbol{z} \in \mathbb{R}^{2d}.$$

If $p(\boldsymbol{z};h)$ depends on a parameter h then we write $p \in S(m)$ if there exists $h_0 > 0$ and constants $C_{\boldsymbol{k}}$ such for all $0 < h < h_0$ the above condition is satisfied.

For example, if $p \in S(1)$ then by Lemma 2.1.2 the operator norm of $\operatorname{op}[p]$ is bounded by a finite linear combination of these $C_{\boldsymbol{k}}$. If $p \in S(m)$ where $m \in L^1(\mathbb{R}^{2d})$ then by Lemma 2.1.3 the trace norm of $\operatorname{op}[p]$ is bounded by a finite linear combination of $C_{\boldsymbol{k}}$.

Notation 2.4.9. We define the semiclassical pseudodifferential operator with Weyl symbol q by

$$\operatorname{op}_h^{\mathrm{W}}[q] := \operatorname{op}_1^{\mathrm{W}}[q(\sqrt{h}\boldsymbol{z})].$$

It is more usual for $\operatorname{op}_h^{\mathrm{W}}[q]$ to denote the operator $\operatorname{op}_1^{\mathrm{W}}[q(\boldsymbol{x}, h\boldsymbol{\xi})]$ as it did in §1.3. However, that operator is unitarily equivalent to the one defined above, so there is no mathematical difference in the choice. The convention used here is more convenient because it avoids the need to separate out $\boldsymbol{x}$ and $\boldsymbol{\xi}$.

Here is the semi-classical composition result that was referred to earlier.

Theorem 2.4.10 (special case of Dimassi and Sjöstrand, 1999, Proposition 7.7)**.** *Let m_1 and m_2 be order functions, and let $p(\boldsymbol{z};h) \in S(m_1)$, $q(\boldsymbol{z};h) \in S(m_2)$. Let $n \in \mathbb{N}_0$. Then*

$$\operatorname{op}_h^{\mathrm{W}}[p(\boldsymbol{z};h)] \operatorname{op}_h^{\mathrm{W}}[q(\boldsymbol{z};h)] = \sum_{j=0}^{n} h^j \operatorname{op}_h^{\mathrm{W}}[F_j(\boldsymbol{z},\boldsymbol{z};h)] + h^{n+1} \operatorname{op}_h^{\mathrm{W}}[R_{n+1}(\boldsymbol{z};h)],$$

where F_j and R_{n+1} were defined in Lemma 2.3.3. Furthermore, for each $j \in \{0,\dots,n\}$ we have $F_j(\boldsymbol{z},\boldsymbol{z};h) \in S(m_1 m_2)$, and $R_{n+1}(\boldsymbol{z};h) \in S(m_1 m_2)$.

More generally, we may prove a semiclassical composition result where p and q have semi-classical expansions (in which case the terms of size h^j for $j < n+1$ have no dependence on h apart from their coefficients). For example, see the book by Robert (1987, Théorème (II-30)). However, this differs from the above result only in the need to collect the various terms of the same asymptotic size; this would only obscure the comparison with the proof of the main result of this thesis.

Remark 2.4.11. As with Theorem 2.4.4, if we restrict attention to $p, q \in \mathscr{S}(\mathbb{R}^{2d})$ with no dependence on h then the final conclusion of Theorem 2.4.10 is trivial, because all Schwartz functions are bounded by all order functions. (However, if p or q depend on h then the conclusion expresses the non-trivial fact that F_j and R_{n+1} and their derivatives are bounded independently of h.) To see this, let $p \in \mathscr{S}(\mathbb{R}^{2d})$, let $\boldsymbol{k} \in \mathbb{N}_0^{2d}$, let m be an order function, and let $\boldsymbol{x}_0 \in \mathbb{R}^{2d}$ such that $m(\boldsymbol{x}_0) \neq 0$;

then there exists a constant $C'_{\boldsymbol{k}}$ such that for all $\boldsymbol{x}\in\mathbb{R}^{2d}$ we have, applying Lemma 2.2.2,

$$|\partial^{\boldsymbol{k}} p(\boldsymbol{x})| \leqslant \frac{C'_{\boldsymbol{k}}}{\langle\boldsymbol{x}\rangle^N} \leqslant \frac{C'_{\boldsymbol{k}}}{\langle\boldsymbol{x}\rangle^N}\frac{C_0\langle\boldsymbol{x}-\boldsymbol{x}_0\rangle^N m(\boldsymbol{x})}{m(\boldsymbol{x}_0)} \leqslant \frac{C'_{\boldsymbol{k}} C_0(\sqrt{2})^N}{\langle\boldsymbol{x}_0\rangle^N m(\boldsymbol{x}_0)} m(\boldsymbol{x}).$$

However, it is again the case that we are able to show a suitable relationship between the constants; that is, we show that

$$\partial_{\boldsymbol{z}}^{\boldsymbol{k}} F_j(\boldsymbol{z},\boldsymbol{z}) \leqslant C_{j,\boldsymbol{k}} m_1(\boldsymbol{z}) m_2(\boldsymbol{z}), \qquad \partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z}) \leqslant C_{n+1,\boldsymbol{k}} m_1(\boldsymbol{z}) m_2(\boldsymbol{z}),$$

where the constants $C_{j,\boldsymbol{k}}$ and $C_{n+1,\boldsymbol{k}}$ depend on p and q only in terms of the constants in their bounds by the order functions m_1 and m_2. As with the symbol classes, this is enough to illustrate how the idea of proving the semiclassical result differs from proving the result of this thesis.

Idea of proof for Theorem 2.4.10. Series and remainder. Define $\tilde{p}(\boldsymbol{z};h) := p(\sqrt{h}\boldsymbol{z};h)$, $\tilde{q}(\boldsymbol{z};h) := q(\sqrt{h}\boldsymbol{z};h)$. Then by Remark 2.3.4 we have

$$\begin{aligned}
\tilde{F}_j(\boldsymbol{x},\boldsymbol{y};h) &= \frac{\mathrm{i}^j}{j!2^j}\sum_{|\boldsymbol{m}|=j}(-1)^{|\boldsymbol{m}_2|}\partial_{\boldsymbol{x}}^{\boldsymbol{m}} p(\sqrt{h}\boldsymbol{x};h)\partial_{\boldsymbol{y}}^{\tau(\boldsymbol{m})} q(\sqrt{h}\boldsymbol{y};h)\\
&= \frac{\mathrm{i}^j}{j!2^j}\sum_{|\boldsymbol{m}|=j}(-1)^{|\boldsymbol{m}_2|}(\sqrt{h})^{|\boldsymbol{m}|+|\tau(\boldsymbol{m})|}(\partial^{\boldsymbol{m}} p)(\sqrt{h}\boldsymbol{x};h)(\partial^{\tau(\boldsymbol{m})} q)(\sqrt{h}\boldsymbol{y};h)\\
&= h^j F_j(\sqrt{h}\boldsymbol{x},\sqrt{h}\boldsymbol{y};h).
\end{aligned}$$

Applying Lemma 2.3.3 to $\tilde{p}$ and $\tilde{q}$, this proves the series expansion and remainder expansion for $\mathrm{op}_h^{\mathrm{W}}[p(\boldsymbol{z};h)]\,\mathrm{op}_h^{\mathrm{W}}[q(\boldsymbol{z};h)]$.

$F_j(\boldsymbol{z},\boldsymbol{z};h)\in S(m_1 m_2)$. Using Remark 2.3.4, for any $\boldsymbol{k}\in\mathbb{N}_0^{2d}$ we have

$$\partial^{\boldsymbol{k}} F_j(\boldsymbol{x},\boldsymbol{y}) = \frac{\mathrm{i}^j}{j!2^j}\sum_{\boldsymbol{l}\leqslant\boldsymbol{k}}\sum_{|\boldsymbol{m}|=j}\binom{\boldsymbol{k}}{\boldsymbol{l}}(-1)^{|\boldsymbol{m}_2|}\partial^{\boldsymbol{m}+\boldsymbol{l}} p(\boldsymbol{x})\partial^{\tau(\boldsymbol{m})+\boldsymbol{k}-\boldsymbol{l}} q(\boldsymbol{y}),$$

so for $0<h<h_0$ (where h_0 is the minimum of the relevant constants for p and q)

$$|\partial^{\boldsymbol{k}} F_j(\boldsymbol{x},\boldsymbol{y};h)| \leqslant \frac{1}{j!2^j}\left(\sum_{\boldsymbol{l}\leqslant\boldsymbol{k}}\sum_{|\boldsymbol{m}|=j}\binom{\boldsymbol{k}}{\boldsymbol{l}} C_{\boldsymbol{m}+\boldsymbol{l}} C'_{\tau(\boldsymbol{m})+\boldsymbol{k}-\boldsymbol{l}}\right) m_1(\boldsymbol{x}) m_2(\boldsymbol{y}).$$

Putting $\boldsymbol{x}=\boldsymbol{y}=\boldsymbol{z}$ shows that $F_j(\boldsymbol{z},\boldsymbol{z};h)\in S(m_1 m_2)$.

$R_{n+1}(\boldsymbol{z};h)\in S(m_1 m_2)$. Choosing $S=N+2d+1$ (where the N is for m_1), for $0<h<h_0$ and any $l\leqslant|\boldsymbol{k}|$ we have

$$\frac{[p]_{n+1+l,T}(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})}{\langle\boldsymbol{x}\rangle^S} \leqslant \frac{[p]_{n+1+l,T}(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})}{\langle\boldsymbol{x}\rangle^{2d+1}\langle\sqrt{t}\boldsymbol{x}\rangle^N} \leqslant \Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+T+|\boldsymbol{k}|} C_{\boldsymbol{r}}\Big)\frac{\langle\sqrt{t}\boldsymbol{x}\rangle^N m_1(\boldsymbol{z})}{\langle\boldsymbol{x}\rangle^{2d+1}\langle\sqrt{t}\boldsymbol{x}\rangle^N}.$$

Substituting this, and the analogous result for q, into Lemma 2.4.2 we obtain

$$|\partial^{\boldsymbol{k}} R_{n+1}(\boldsymbol{z};h)| \leqslant C_{\boldsymbol{k},n,S,T}\Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+T+|\boldsymbol{k}|} C_{\boldsymbol{r}}\Big)\Big(\max_{n+1\leqslant|\boldsymbol{r}|\leqslant n+1+S+|\boldsymbol{k}|} C'_{\boldsymbol{r}}\Big)|\boldsymbol{k}| I^2 m_1(\boldsymbol{z}) m_2(\boldsymbol{z}),$$

where I is the integral of $1/\langle\boldsymbol{z}\rangle^{2d+1}$ and $C_{\boldsymbol{k},n,S,T}$ is the constant from Lemma 2.4.2. □

Chapter 3

Functions of pseudodifferential operators

In Chapter 2 we investigated the composition of Weyl pseudodifferential operators; that is,

$$\mathrm{op}[p]\,\mathrm{op}[q] \approx \mathrm{op}[pq].$$

This chapter is concerned with approximating functions of pseudodifferential operators; that is,

$$f(\mathrm{op}[q]) \approx \mathrm{op}[f(q)].$$

The close relationship between these two approximations can be seen by taking $f(t) = t^2$ and $p = q$, in which case the two approximate equations are the same. Indeed, the main result of this chapter is an explicit trace norm bound for $f(\mathrm{op}[q]) - \mathrm{op}[f(q)]$, which is proved by just combining a more general bound with the trace norm bound for composition from the previous chapter. This type of argument is standard and the author makes no claim of novelty. However, existing results of this type are usually expressed in terms of the particular composition bound being used, so are not directly applicable here. In contrast, in this chapter, the results for functions of operators are not combined with the composition bound until the last possible moment.

We begin with some technical details in §3.1, where we discuss derivatives and integrals of operator-valued functions. We apply this in §3.2, where for self-adjoint operators we prove a bound in terms of $\|\mathrm{op}[q]\,\mathrm{op}[\mathrm{e}^{\mathrm{i}tq}] - \mathrm{op}[q\mathrm{e}^{\mathrm{i}tq}]\|_1$. In §3.3 we prove a result for general operators, but where the function f must be complex-analytic, with a bound expressed in terms of $\|\mathrm{op}[q^k]\,\mathrm{op}[q] - \mathrm{op}[q^{k+1}]\|_1$. Finally, in §3.4, we combine these results with the trace norm bound proved in §2.3 to give a bound for the functional approximation in terms of F_1 (which was defined in Lemma 2.3.3).

3.1 Operator-valued functions

In §3.2 we will use information about the composition of operators to give information about functions of self-adjoint operators. To do this we will need to differentiate and integrate operator-valued functions. In this section we define the derivative of such functions and discuss its basic properties, then define the integral of such functions and discuss its properties, finishing with a version of the fundamental theorem of calculus that relates them. We will use the notation $\mathscr{B}(\mathscr{H})$ for the algebra of bounded operators on a Hilbert space $\mathscr{H}$, and we will simply denote $\mathscr{S}(\mathbb{R}^d)$ and $L^2(\mathbb{R}^d)$ by $\mathscr{S}$ and L^2 respectively.

The derivative for operator-valued functions on the real numbers is defined in the same way as for scalar-valued functions, with the limit taken in the operator norm.

Definition 3.1.1. Let $t \in \mathbb{R}$ and let $F \colon \mathbb{R} \to \mathscr{B}(\mathscr{H})$ be a function such that an operator $A \in \mathscr{B}(\mathscr{H})$ exists satisfying

$$\left\| A - h^{-1}\big(F(t+h) - F(t)\big) \right\| \to 0$$

as $h \to 0$. Then we say that F is differentiable at t and denote $F'(t) := A$.

Differentiation is linear in the function and satisfies the product rule for compositions of operators (see Lang, 1993, Chapter XIII). There are two cases in which we will need sufficient conditions for differentiability and an explicit expression for the derivative. The first of these is that the operator-valued function is unitarily equivalent to a family of multiplication operators, which is covered by the following remark and lemma.

Remark 3.1.2. If $A \colon \mathscr{H}_1 \to \mathscr{H}_2$ is a bounded invertible operator between Hilbert spaces and $F \colon \mathbb{R} \to \mathscr{B}(\mathscr{H}_1)$ is a differentiable function, then $A^{-1}FA \colon \mathbb{R} \to \mathscr{B}(\mathscr{H}_2)$ is a differentiable function and, for each $t \in \mathbb{R}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(A^{-1}F(t)A\big) = A^{-1}F'(t)A.$$

This follows immediately from the product rule and the fact that $\frac{\mathrm{d}}{\mathrm{d}t}A = 0$.

Lemma 3.1.3. *Let (M,η) be a measure space. Let $g \colon M \times \mathbb{R} \to \mathbb{C}$ be twice continuously differentiable in the second variable such that for each $t \in \mathbb{R}$ we have $g(\boldsymbol{x};t), \frac{\partial}{\partial t}g(\boldsymbol{x};t), \frac{\partial^2}{\partial t^2}g(\boldsymbol{x};t) \in L^\infty(M,\eta)$, and there exists an interval I containing t for which*

$$\sup_{\boldsymbol{x}\in M}\sup_{s\in I}\left|\frac{\partial^2}{\partial s^2}g(\boldsymbol{x};s)\right| < \infty.$$

Let F be the function taking values in $\mathscr{B}(L^2)$ given by multiplication by $g(\boldsymbol{x};t)$ for each $t \in \mathbb{R}$ i.e.

$$\big(F(t)u\big)(\boldsymbol{x}) = g(\boldsymbol{x};t)u(\boldsymbol{x}), \quad \boldsymbol{x} \in M.$$

Then F is differentiable, and

$$\big(F'(t)u\big)(\boldsymbol{x}) = \Big(\frac{\partial}{\partial t}g(\boldsymbol{x};t)\Big)u(\boldsymbol{x}), \quad \boldsymbol{x} \in M.$$

Proof. Let $\mathscr{M}(a(\boldsymbol{x}))$ denote the operator of multiplication by a function $a(\boldsymbol{x})$, which satisfies $\|\mathscr{M}(a(\boldsymbol{x}))\| = \|a\|_{L^\infty(M,\mu)}$. Thus, by Taylor's theorem,

$$
\begin{aligned}
&\left\|\mathscr{M}\Big(\frac{\partial}{\partial t}g(\boldsymbol{x};t)\Big) - h^{-1}\big(\mathscr{M}(g(\boldsymbol{x};t+h)) + \mathscr{M}(g(\boldsymbol{x};t))\big)\right\| \\
&= \left\|\mathscr{M}\Big(\frac{\partial}{\partial t}g(\boldsymbol{x};t) - h^{-1}\big(g(\boldsymbol{x};t+h) + g(\boldsymbol{x};t)\big)\Big)\right\| \\
&= \left\|\frac{\partial}{\partial t}g(\boldsymbol{x};t) - h^{-1}\big(g(\boldsymbol{x};t+h) + g(\boldsymbol{x};t)\big)\right\|_{L^\infty(M,\eta)} \\
&= \left\|\frac{1}{h}h^2\int_0^1 (1-s)\frac{\partial^2}{\partial t^2}g(\boldsymbol{x};t+sh)\,\mathrm{d}s\right\|_{L^\infty(M,\eta)} \\
&\leqslant \frac{h}{2}\sup_{\boldsymbol{x}\in M}\sup_{|r|<|h|}\left|\frac{\partial^2}{\partial t^2}g(\boldsymbol{x};t+r)\right| \\
&\to 0 \qquad \text{as } h\to 0.
\end{aligned}
$$

□

The other type of operator-valued function that we will need to differentiate is one expressed in terms of a parametrised collection of Weyl pseudodifferential operator symbols. This is dealt with by the next lemma.

Lemma 3.1.4. *Let $q \in C^\infty(\mathbb{R}^{2d}\times\mathbb{R})$ such that $q(\boldsymbol{z},t), \frac{\partial}{\partial t}q(\boldsymbol{z},t), \frac{\partial^2}{\partial t^2}q(\boldsymbol{z},t) \in C_{\mathrm{b}}^\infty(\mathbb{R}^{2d})$ for all $t\in\mathbb{R}$ and such that, for each $t\in\mathbb{R}$ and multi-index $\boldsymbol{k}\in\mathbb{N}_0^{2d}$, there exists an open interval $I_{\boldsymbol{k}}$ containing t where*

$$
\sup_{\boldsymbol{z}\in\mathbb{R}^{2d}}\sup_{s\in I_{\boldsymbol{k}}}\left|\frac{\partial^2}{\partial s^2}\partial_{\boldsymbol{z}}^{\boldsymbol{k}}q(\boldsymbol{z};s)\right| < \infty.
$$

Then $t\mapsto \operatorname{op}[q(\boldsymbol{z};t)]$ is a differentiable function, and

$$
\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{op}[q(\boldsymbol{z};t)] = \operatorname{op}\Big[\frac{\partial}{\partial t}q(\boldsymbol{z};t)\Big].
$$

Proof. We must show that $\lim_{h\to 0}\|A(h)\| = 0$, where

$$
A(h) := \frac{1}{h}\big(\operatorname{op}[q(\boldsymbol{z};t+h)] - \operatorname{op}[q(\boldsymbol{z};t)]\big) - \operatorname{op}\Big[\frac{\partial}{\partial t}q(\boldsymbol{z};t)\Big].
$$

But op is linear in the symbol, so by Taylor's theorem

$$
\begin{aligned}
A(h) &= \operatorname{op}\Big[\frac{1}{h}\Big(q(\boldsymbol{z};t+h) - q(\boldsymbol{z};t) - h\frac{\partial}{\partial t}q(\boldsymbol{z};t)\Big)\Big] \\
&= -\operatorname{op}\Big[\frac{1}{h}\Big(h^2\int_0^1(1-s)\frac{\partial^2}{\partial t^2}q(\boldsymbol{z};t+sh)\,\mathrm{d}s\Big)\Big].
\end{aligned}
$$

So by Lemma 2.1.2,

$$
\begin{aligned}
\|A(h)\| &\leqslant C_d \max_{|\boldsymbol{k}|\leqslant d+2}\sup_{\boldsymbol{z}\in\mathbb{R}^{2d}}\left|h\int_0^1(1-s)\frac{\partial^2}{\partial t^2}\partial_{\boldsymbol{z}}^{\boldsymbol{k}}q(\boldsymbol{z};t+sh)\,\mathrm{d}s\right| \\
&\leqslant hC_d \max_{|\boldsymbol{k}|\leqslant d+2}\sup_{\boldsymbol{z}\in\mathbb{R}^{2d}}\max_{|r|<|h|}\left|\frac{\partial^2}{\partial t^2}\partial_{\boldsymbol{z}}^{\boldsymbol{k}}q(\boldsymbol{z};t+r)\right| \\
&\to 0 \qquad \text{as } h\to 0.
\end{aligned}
$$

□

We now recall the properties of integrals of operator-valued functions. It is possible to define the Lebesgue integral for such functions in exactly the same way as for scalar-valued functions, by starting with simple functions and using a density argument (see, for example, Lang, 1993, Chapter VI); this is usually called the *Bochner integral*. For any $u, v \in L^2$ this integral of a $\mathscr{B}(L^2)$-valued function F satisfies (see Lang, 1993, Chapter VI, Theorem 4.1)

$$\left\langle \int F(t)\,\mathrm{d}t\, u, v \right\rangle = \int \langle F(t)u, v\rangle\,\mathrm{d}t.$$

For our purposes it will be more convenient to define the integral of F by this identity, as follows. This weaker type of integration is usually called the *Pettis integral* (see Curtain and Zwart, 1995, Definition A.5.11).

Definition 3.1.5 (Pettis integral)**.** Let $E \subseteq \mathbb{R}$ be a measurable set, let $\mathscr{H}$ be a separable Hilbert space, and let $F : \mathbb{R} \to \mathscr{B}(\mathscr{H})$ be an operator-valued function such that for each $u, v \in \mathscr{H}$ the function $\langle F(t)u, v\rangle$ is integrable (in particular, measurable) on E. Then we say that $F(t)$ is integrable on E. Furthermore, there exists a bounded operator $A \in \mathscr{B}(\mathscr{H})$ satisfying

$$\langle Au, v\rangle = \int_E \langle F(t)u, v\rangle\,\mathrm{d}t$$

for all $u, v \in \mathscr{H}$ (see Curtain and Zwart, 1995, Theorem A.5.10), and A is the unique operator satisfying this because an operator is determined by its bilinear form (see Birman and Solomjak, 1987, Theorem 2.4.6); we call A the integral of $F(t)$ on E.

As with differentiation, there are two cases in which we need sufficient conditions for integrability and explicit expressions for the integral. The first is again that the function is unitarily equivalent to multiplication by a parametrised family of functions, which is dealt with by the next lemma.

Lemma 3.1.6. *Let (M, η) be a measure space. Let $g : M \times \mathbb{R} \to \mathbb{C}$ be a measurable function and let $T : L^2(\mathbb{R}^d) \to L^2(M, \eta)$ be a unitary operator. Set*

$$F(t) := T^* g(\boldsymbol{x}, t) T,$$

where for each $t \in \mathbb{R}$ the function $\boldsymbol{x} \mapsto g(\boldsymbol{x}, t)$ acts on $L^2(M, \eta)$ by multiplication. If there exists a non-negative function $h \in L^1(\mathbb{R})$ such that $|g(t, \boldsymbol{x})| \leqslant h(t)$ for each $\boldsymbol{x} \in M$ and $t \in \mathbb{R}$ then F is integrable and

$$\int_{\mathbb{R}} F(t)\,\mathrm{d}t = T^* \int_{\mathbb{R}} g(\boldsymbol{x}, t)\,\mathrm{d}t\, T,$$

where the function $\boldsymbol{x} \mapsto \int_{\mathbb{R}} g(\boldsymbol{x}, t)\,\mathrm{d}t$ on M acts by multiplication.

Proof. First note that

$$\int_{\mathbb{R}} \langle F(t)u, v\rangle_{L^2(\mathbb{R}^d)}\,\mathrm{d}t = \int_{\mathbb{R}} \langle g(\boldsymbol{x}, t)Tu, Tv\rangle_{L^2(M,\eta)}\,\mathrm{d}t = \int_{\mathbb{R}} \int_M g(\boldsymbol{x}, t)Tu(\boldsymbol{x})\overline{Tv(\boldsymbol{x})}\,\eta(\mathrm{d}\boldsymbol{x})\,\mathrm{d}t.$$

By Hölder's inequality the product $(Tu)(Tv)$ is absolutely integrable, and so bounding $|g(\boldsymbol{x},t)|$ by $h(t)$ we find that the integrand is absolutely integrable on $M\times\mathbb{R}$ with the measure $\eta\times\mu_1$. This proves that F is integrable. To find the expression for its integral, we may apply Fubini's theorem, so that

$$\int_{\mathbb{R}}\langle F(t)u,v\rangle_{L^2(\mathbb{R}^{2d})}\,\mathrm{d}t=\int_M\Big(\int_{\mathbb{R}}g(\boldsymbol{x},t)\,\mathrm{d}t\Big)Tu(\boldsymbol{x})\overline{Tv(\boldsymbol{x})}\eta(\mathrm{d}\boldsymbol{x})=\Big\langle\int_{\mathbb{R}}g(\boldsymbol{x},t)\,\mathrm{d}t\,Tu,Tv\Big\rangle_{L^2(M,\eta)}.$$

Thus the integral of F equals $T^*\int g(\boldsymbol{x},t)\,\mathrm{d}t\,T$. □

As with differentiation, the other case of interest is where the function is expressed in terms of a parametrised collection of Weyl pseudodifferential operator symbols.

Lemma 3.1.7. *Let $q\in C^\infty(\mathbb{R}^{2d}\times\mathbb{R})$ such that, for each multi-index $\boldsymbol{k}\in\mathbb{N}_0^{2d}$, there exists a bounded non-negative function $h_{\boldsymbol{k}}\in L^1(\mathbb{R})$ such that*

$$|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}q(\boldsymbol{z};t)|\leqslant h_{\boldsymbol{k}}(t)\qquad\forall\boldsymbol{z}\in\mathbb{R}^{2d},t\in\mathbb{R}.$$

Then $\mathrm{op}[q(\boldsymbol{z};t)]$ *is an integrable operator-valued function on $t\in\mathbb{R}$, and its integral satisfies*

$$\int_{\mathbb{R}}\mathrm{op}[q(\boldsymbol{z};t)]\,\mathrm{d}t=\mathrm{op}\Big[\int_{\mathbb{R}}q(\boldsymbol{z};t)\,\mathrm{d}t\Big].$$

Proof. We will first show that the operator on each side of this identity is well-defined and bounded. Then we will show that they are equal on $\mathscr{S}$, and finally use the density of $\mathscr{S}$ in L^2 to show that they are equal on L^2.

$\underline{\mathrm{op}[q(\boldsymbol{z};t)]\text{ is integrable.}}$ For each $t\in\mathbb{R}$ we have, by Lemma 2.1.2,

$$\|\mathrm{op}[q(\boldsymbol{z};t)]\|\leqslant C_d\max_{|\boldsymbol{k}|\leqslant d+2}\|\partial^{\boldsymbol{k}}q(\boldsymbol{z};t)\|_{L^\infty(\mathbb{R}^{2d})}\leqslant C_d\max_{|\boldsymbol{k}|\leqslant d+2}h_{\boldsymbol{k}}(t),$$

so

$$\int_{\mathbb{R}}\|\mathrm{op}[q(\boldsymbol{z};t)]\|\,\mathrm{d}t\leqslant C_d\int_{\mathbb{R}}\max_{|\boldsymbol{k}|\leqslant d+2}h_{\boldsymbol{k}}(t)\,\mathrm{d}t\leqslant C_d\int_{\mathbb{R}}\sum_{|\boldsymbol{k}|\leqslant d+2}h_{\boldsymbol{k}}(t)\,\mathrm{d}t=C_d\sum_{|\boldsymbol{k}|\leqslant d+2}\int_{\mathbb{R}}h_{\boldsymbol{k}}(t)\,\mathrm{d}t.$$

This is finite because each $h_{\boldsymbol{k}}$ is integrable, so it follows that $\mathrm{op}[q(\boldsymbol{z};t)]$ is integrable.

$\underline{\mathrm{op}\big[\int q(\boldsymbol{z};t)\,\mathrm{d}t\big]\text{ is a bounded operator.}}$ We may differentiate under the integral because q is smooth and each derivative in $\boldsymbol{z}$ is bounded by an integrable function $h_{\boldsymbol{k}}$ (see Lang, 1993, Chapter XIII, Lemma 2.2); therefore, for every $\boldsymbol{z}\in\mathbb{R}^{2d}$,

$$\Big|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}\int_{\mathbb{R}}q(\boldsymbol{z};t)\,\mathrm{d}t\Big|=\Big|\int_{\mathbb{R}}\partial^{\boldsymbol{k}}q(\boldsymbol{z};t)\,\mathrm{d}t\Big|\leqslant\int_{\mathbb{R}}|\partial^{\boldsymbol{k}}q(\boldsymbol{z};t)|\,\mathrm{d}t\leq\int_{\mathbb{R}}h_{\boldsymbol{k}}(t)\,\mathrm{d}t.$$

By Lemma 2.1.2 the operator $\mathrm{op}\big[\int q(\boldsymbol{z};t)\,\mathrm{d}t\big]$ is therefore well-defined on L^2 with

$$\Big\|\mathrm{op}\Big[\int_{\mathbb{R}}q(\boldsymbol{z};t)\,\mathrm{d}t\Big]\Big\|\leqslant C_d\max_{|\boldsymbol{k}|\leqslant d+2}\int_{\mathbb{R}}h_{\boldsymbol{k}}(t)\,\mathrm{d}t.$$

Bilinear forms on $\mathscr{S}\times\mathscr{S}$. We have shown that $\int \operatorname{op}[q(\boldsymbol{z};t)]\,\mathrm{d}t$ and $\operatorname{op}\big[\int q(\boldsymbol{z};t)\,\mathrm{d}t\big]$ are are well-defined and bounded operators. It remains to show that they are equal. To do so we first show that the bilinear forms corresponding to the two operators agree on $\mathscr{S}\times\mathscr{S}$. Let $u, v\in\mathscr{S}$, and note that

$$\left\langle \operatorname{op}\left[\int_{\mathbb{R}} q(\boldsymbol{z};t)\,\mathrm{d}t\right]u, v\right\rangle = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{\xi}} q\big(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}),\boldsymbol{\xi};t\big)u(\boldsymbol{y})\overline{v(\boldsymbol{x})}\,\mathrm{d}t\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{x}.$$

Denote the integrand of this expression by $f(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi};t)$. This is an iterated integral and it is not immediately clear that we can interchange the order of integration. We interchange the $\mathrm{d}t$ integral with the one outside of it one step at a time:

1. We may bound $|f(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi};t)| \leqslant h_{\boldsymbol{0}}(t)|u(\boldsymbol{y})||v(\boldsymbol{x})|$. This is absolutely integrable in $(t,\boldsymbol{y})$ (because $u\in\mathscr{S}$) so by Fubini's theorem we may interchange the $\mathrm{d}t$ integral with the $\mathrm{d}\boldsymbol{y}$ integral.

2. To interchange the $\mathrm{d}t$ integral with the $\mathrm{d}\boldsymbol{\xi}$ integral we must show that $\int f(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi};t)\,\mathrm{d}\boldsymbol{y}$ is absolutely integrable as a function of $\boldsymbol{\xi}$ and t. The decay in $\boldsymbol{\xi}$ follows in precisely the same way as in Lemma 2.2.5, and the decay in t comes from bounding derivatives of q by $h_{\boldsymbol{k}}$.

3. Finally, to swap the order of integration of $\boldsymbol{x}$ and t we proceed in the same way as the third part of Lemma 2.2.5, and bound $\partial^{\boldsymbol{k}}q$ by $h_{\boldsymbol{k}}$ to show that we may apply Fubini's theorem.

We therefore have

$$\begin{aligned}\left\langle \operatorname{op}\left[\int q(\boldsymbol{z};t)\,\mathrm{d}t\right]u, v\right\rangle &= \frac{1}{(2\pi)^d}\int_{\mathbb{R}}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{\xi}} q\big(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}),\boldsymbol{\xi};t\big)u(\boldsymbol{y})\overline{v(\boldsymbol{x})}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t\\ &= \int \langle \operatorname{op}[q(\boldsymbol{z};t)]u, v\rangle\,\mathrm{d}t.\end{aligned}$$

General functions in L^2. For $u, v\in L^2$ let

$$B(u,v) := \left\langle \int_{\mathbb{R}} \operatorname{op}[q(\boldsymbol{z};t)]\,\mathrm{d}t\; u, v\right\rangle - \left\langle \operatorname{op}\left[\int_{\mathbb{R}} q(\boldsymbol{z};t)\,\mathrm{d}t\right]u, v\right\rangle.$$

This is a bounded bilinear form on $L^2\times L^2$ because it is the difference of two bounded bilinear forms, and we have shown that it is identically zero on $\mathscr{S}\times\mathscr{S}$. For each $u\in L^2$ and $v\in\mathscr{S}$ we may approximate u by $\tilde{u}\in\mathscr{S}$, with

$$|B(u,v) - B(\tilde{u},v)| \leqslant \|B\|\,\|u-\tilde{u}\|_{L^2}\|v\|_{L^2},$$

which may be made arbitrarily small, so in fact B is zero on $L^2\times\mathscr{S}$. By the same argument it is zero on $L^2\times L^2$, so its corresponding operator is zero (Birman and Solomjak, 1987, Theorem 2.4.6). We have therefore shown that $\int \operatorname{op}[q(\boldsymbol{z};t)]\,\mathrm{d}t = \operatorname{op}\big[\int q(\boldsymbol{z};t)\,\mathrm{d}t\big]$. □

In the next section, we bound the trace norm of functions of operators by writing them as integrals of operator-valued functions. The final step is therefore the application of the next lemma, which bounds the trace norm of an integral in terms of its integrand.

Lemma 3.1.8. *Let $F : \mathbb{R} \to \mathscr{B}(L^2)$ be a measurable function such that $\|F(t)\|_1$ is integrable. Then the integral of F is a trace class operator with*

$$\left\| \int_{\mathbb{R}} F(t)\,\mathrm{d}t \right\|_1 \leqslant \int_{\mathbb{R}} \|F(t)\|_1\,\mathrm{d}t.$$

Proof. For all orthonormal sequences $u_j, v_j \in L^2(\mathbb{R}^d)$ we have

$$\sum_j \left| \left\langle \int_{\mathbb{R}} F(t)\,\mathrm{d}t\, u_j, v_j \right\rangle \right| = \sum_j \left| \int_{\mathbb{R}} \langle F(t)u_j, v_j\rangle\,\mathrm{d}t \right| \leqslant \sum_j \int_{\mathbb{R}} |\langle F(t)u_j, v_j\rangle|\,\mathrm{d}t.$$

We may interchange the order of integration (considering the sum as an integral with the counting measure) because the integrand is non-negative, so

$$\sum_j \left| \left\langle \int_{\mathbb{R}} F(t)\,\mathrm{d}t\, u_j, v_j \right\rangle \right| \leqslant \int_{\mathbb{R}} \sum_j |\langle F(t)u_j, v_j\rangle|\,\mathrm{d}t.$$

But the sum in this expression is bounded by the trace norm of $F(t)$ (see Birman and Solomjak, 1987, Theorem 11.2.3). Since this holds for all orthonormal sequences, $\int F(t)\,\mathrm{d}t$ is trace class with the stated trace norm bound (see Birman and Solomjak, 1987, Theorem 11.2.3 and Theorem 11.2.4). □

Finally, we relate the derivative and integral with the fundamental theorem of calculus. To prove it, we use the common trick of just reducing it to the scalar-valued case.

Theorem 3.1.9 (Fundamental theorem of calculus)**.** *Let $a, b \in \mathbb{R}$ and let $F : \mathbb{R} \to \mathscr{B}(L^2)$ be continuously differentiable on $[a, b]$. Then $F'(t)$ is integrable on $[a, b]$, and*

$$\int_a^b F'(t)\,\mathrm{d}t = F(b) - F(a).$$

Proof. We have (see Lang, 1993, Corollary XIII.3.2)

$$\langle F'(t)u, v\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle F(t)u, v\rangle,$$

so by the scalar-valued fundamental theorem of calculus

$$\int_a^b \langle F'(t)u, v\rangle\,\mathrm{d}t = \int_a^b \frac{\mathrm{d}}{\mathrm{d}t}\langle F(t)u, v\rangle\,\mathrm{d}t = \langle (F(b) - F(a))u, v\rangle.$$

Thus $F'(t)$ is integrable on $[a, b]$ with integral equal to $F(b) - F(a)$. □

3.2 Functions of self-adjoint operators

For a bounded self-adjoint operator A acting on $L^2(\mathbb{R}^d)$ and a suitable function f it is possible to assign meaning to the expression $f(A)$. Specifically, the spectral theorem says that there is a unitary operator $T : L^2(\mathbb{R}^d) \to L^2(M, \mu)$ and a real-valued function $a \in L^\infty(M, \mu)$ such that $A = T^* a T$ (see for example Berezin and Shubin, 1991, §S1.1), and we define

$$f(A) := T^* f(a) T.$$

This is unique in the sense that if A is expressed in a similar way with another unitary operator and function, then $f(A)$ defined in the analogous way gives rise to the same operator as the one defined in terms of T and a.

We will be concerned with showing that, in a suitable sense,

$$f(\mathrm{op}[q]) \approx \mathrm{op}[f(q)].$$

To obtain the above approximate relationship we will write f in terms of its Fourier transform, so that

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]} \hat{f}(t)\,\mathrm{d}t \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{op}[\mathrm{e}^{\mathrm{i}tq}] \hat{f}(t)\,\mathrm{d}t.$$

The operator $\mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]}$ is also defined using the spectral theorem, and satisfies

$$\mathrm{i}\,\mathrm{op}[q] \mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]} = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]},$$

so we may obtain information about $f(\mathrm{op}[q])$ by investigating the approximate composition relationship

$$\mathrm{i}\,\mathrm{op}[q]\,\mathrm{op}[\mathrm{e}^{\mathrm{i}tq}] \approx \mathrm{op}[\mathrm{i}q\mathrm{e}^{\mathrm{i}tq}].$$

It is a common practice to approximate $\mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]}$, known as the *propagator*, by a pseudodifferential operator, or more generally an operator whose Schwartz kernel is an oscillatory integral; see for example the book by Safarov and Vassiliev (1996, Chapter 3) and the book by Shubin (2001, §20). More specifically, the approach in this section is very similar to that of Widom (1982, remarks after equation (7)) and Sobolev (2013, proof of Lemma 12.6), but we will need to bound the trace norm of $f(\mathrm{op}[q]) - \mathrm{op}[f(q)]$ in terms of composition of $\mathrm{op}[q]$ and $\mathrm{op}[\mathrm{e}^{\mathrm{i}tq}]$, which neither of those authors quite make explicit.

We begin with the standard properties of the propagator, which are easily checked.

Lemma 3.2.1. *Let A be a bounded self-adjoint operator on $L^2(\mathbb{R}^d)$ and let $U(t) := \mathrm{e}^{\mathrm{i}tA}$. Then $U(t)$ is infinitely differentiable and satisfies*

$$U(0) = I_{L^2}, \qquad \frac{\mathrm{d}^n}{\mathrm{d}t^n} U(t) = (\mathrm{i}A)^n \mathrm{e}^{\mathrm{i}tA}.$$

Additionally, for all $t \in \mathbb{R}$, we have the properties

$$\|U(t)\| = 1, \qquad (U(t))^{-1} = U(-t) \qquad AU(t) = U(t)A.$$

Furthermore, if $f \in \mathscr{S}(\mathbb{R})$ then $\hat{f}(t)U(t)$ is integrable, and

$$\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t) U(t)\,\mathrm{d}t = f(A).$$

Proof. Value at zero and derivative. By the spectral theorem we may write $U(t) = T^*\mathrm{e}^{\mathrm{i}ta}T$ where $a \in L^\infty(M,\eta)$. This immediately implies that

$$U(0) = T^*T = I_{L^2}.$$

We have

$$\frac{\partial^n}{\partial t^n}\mathrm{e}^{\mathrm{i}ta(\boldsymbol{x})} = (\mathrm{i}a(\boldsymbol{x}))^n\mathrm{e}^{\mathrm{i}ta(\boldsymbol{x})},$$

which is bounded on $(\boldsymbol{x},t) \in M \times \mathbb{R}$, so by Remark 3.1.2 and Lemma 3.1.3 we have

$$U'(t) = T^*\frac{\partial}{\partial t}\mathrm{e}^{\mathrm{i}ta}T = T^*\mathrm{i}a\mathrm{e}^{\mathrm{i}ta}T = \mathrm{i}T^*aTT^*\mathrm{e}^{\mathrm{i}ta}T = \mathrm{i}AU(t),$$

and similarly for higher derivatives.

Other properties. We also have

$$\|U(t)\| = \|T^*\mathrm{e}^{\mathrm{i}ta}T\| = \|\mathrm{e}^{\mathrm{i}ta}\|_{L^\infty(M,\eta)} = 1.$$

For the invertibility of U, note that

$$U(t)U(-t) = T^*\mathrm{e}^{\mathrm{i}ta}TT^*\mathrm{e}^{-\mathrm{i}ta}T = T^*\mathrm{e}^0T = T^*T = I_{L^2},$$

and similarly $U(-t)U(t) = I_{L^2}$, so $(U(t))^{-1} = U(-t)$. For the final property we have

$$AU(t) = T^*aTT^*\mathrm{e}^{\mathrm{i}ta}T = T^*a\mathrm{e}^{\mathrm{i}ta}T = T^*\mathrm{e}^{\mathrm{i}ta}TT^*aT = U(t)A.$$

Integral of $\hat{f}(t)U(t)$. We have

$$\hat{f}(t)U(t) = \hat{f}(t)T^*\mathrm{e}^{\mathrm{i}ta}T = T^*\hat{f}(t)\mathrm{e}^{\mathrm{i}ta}T,$$

and the function $\hat{f}(t)\mathrm{e}^{\mathrm{i}ta(\boldsymbol{x})}$ is bounded by $|\hat{f}(t)|$ for all $t \in \mathbb{R}$, $\boldsymbol{x} \in M$, so by Lemma 3.1.6 the product is integrable and we have

$$\int_{\mathbb{R}}\hat{f}(t)U(t)\,\mathrm{d}t = \frac{1}{\sqrt{2\pi}}T^*\int_{\mathbb{R}}\hat{f}(t)\mathrm{e}^{\mathrm{i}ta}\,\mathrm{d}t\,T = T^*f(a)T = f(A). \qquad \square$$

We now prove the analogous properties for $\mathrm{op}[\mathrm{e}^{\mathrm{i}tq}]$, which follow in much the same way.

Lemma 3.2.2. *Let $q \in C_\mathrm{b}^\infty(\mathbb{R}^{2d})$ be real-valued and set $E(t) := \mathrm{op}[\mathrm{e}^{\mathrm{i}tq}]$. Then $E(t)$ is infinitely differentiable and satisfies*

$$E(0) = I_{L^2(\mathbb{R}^d)}, \qquad \frac{\mathrm{d}^n}{\mathrm{d}t^n}E(t) = \mathrm{op}[(\mathrm{i}q)^n\mathrm{e}^{\mathrm{i}tq}].$$

Furthermore, if $f \in \mathscr{S}(\mathbb{R})$ then $\hat{f}(t)E(t)$ is integrable, and

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\hat{f}(t)E(t)\,\mathrm{d}t = \mathrm{op}[f(q)].$$

Proof. Derivatives of $\mathrm{e}^{\mathrm{i}tq}$. Let $l, n \in \mathbb{N}_0$. We have

$$\partial_t^n\Big((q(\boldsymbol{z}))^l \mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}\Big) = (q(\boldsymbol{z}))^{l+n} \mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}.$$

But we also have, for any smooth function r on $\mathbb{R}^{2d}$ and $m \in \{1, \ldots, 2d\}$,

$$\partial_{z_m}\big(r(\boldsymbol{z})\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}\big) = \big(\partial_{z_m} r(\boldsymbol{z})\big)\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})} + \mathrm{i}t\, r(\boldsymbol{z})\big(\partial_{z_m} q(\boldsymbol{z})\big)\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}.$$

By induction, for any multi-index $\boldsymbol{k} \in \mathbb{N}_0^{2d}$, we therefore have

$$\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_t^n\Big((q(\boldsymbol{z}))^l \mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}\Big)\Big) = \mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})} \sum_{j=0}^{|\boldsymbol{k}|} t^j\, r_{j,\boldsymbol{k},l,n}(\boldsymbol{z}),$$

where each $r_{j,\boldsymbol{k},l,n}$ is a linear combination of products of $j+l+n$ factors, and each factor is of the form $\partial^{\boldsymbol{m}} q(\boldsymbol{z})$ with $\boldsymbol{m} \leqslant \boldsymbol{k}$.

Value at zero and derivative of $E(t)$. The fact that $E(0)$, i.e. op[1], is the identity follows from the Fourier inversion theorem and the definition of the Weyl quantisation. To find the derivative, use the expression for the derivative of $\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}$ (with $l = 0$) to bound

$$|\partial_{\boldsymbol{z}}^{\boldsymbol{k}} \partial_t^n \mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}| \leqslant \sum_{j=0}^{|\boldsymbol{k}|} |t|^j |r_{j,\boldsymbol{k},0,n}(\boldsymbol{z})|.$$

This implies that $\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})} \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ for each $t \in \mathbb{R}$, and that the conditions of Lemma 3.1.4 are satisfied for $E(t)$ (e.g. take $I_{\boldsymbol{k}} = (t-1, t+1)$) and so it is differentiable with the stated derivative. Doing the same with $l = 1$ we see that $E'(t)$ is also differentiable, and continuing inductively we find that it is infinitely differentiable.

Integral of $\hat{f}(t)E(t)$. We have $\hat{f}(t)E(t) = \mathrm{op}[\hat{f}(t)\mathrm{e}^{\mathrm{i}tq}]$, so its Weyl symbol is smooth, and using the above expression for the derivative we have

$$|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}(\hat{f}(t)\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})})| = |\hat{f}(t)||\partial_{\boldsymbol{z}}^{\boldsymbol{k}}(\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})})| \leqslant |\hat{f}(t)| \sum_{j=0}^{|\boldsymbol{k}|} |t|^j\, |r_{j,\boldsymbol{k},0,0}(\boldsymbol{z})|.$$

We may bound $|r_{j,\boldsymbol{k},0,0}(\boldsymbol{z})| \leqslant C_{\boldsymbol{k}}$ where $C_{\boldsymbol{k}}$ is a number not dependent on j or $\boldsymbol{z}$, and because $\hat{f} \in \mathscr{S}(\mathbb{R})$ this means that the right hand side is bounded by an integrable function of t. Therefore the hypotheses of Lemma 3.1.7 are satisfied, so $\hat{f}(t)E(t)$ is an integrable function, with

$$\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t)E(t)\,\mathrm{d}t = \mathrm{op}\Big[\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(t)\mathrm{e}^{\mathrm{i}tq(\boldsymbol{z})}\,\mathrm{d}t\Big] = \mathrm{op}[f(q)]. \qquad \square$$

We have established the necessary properties of $\mathrm{e}^{\mathrm{i}t\,\mathrm{op}[q]}$ and $\mathrm{op}[\mathrm{e}^{\mathrm{i}tq}]$. Now, as promised at the start of the section, we will use these to bound the difference in trace norm between $f(\mathrm{op}[q])$ and $\mathrm{op}[f(q)]$.

Lemma 3.2.3. *Let $f \in \mathscr{S}(\mathbb{R})$ and let $q \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$. Then*

$$\|f(\mathrm{op}[q])-\mathrm{op}[f(q)]\|_1 \leqslant \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\left(\int_{[0,t]}\|\mathrm{op}[\mathrm{e}^{\mathrm{i}sq}]\,\mathrm{op}[q]-\mathrm{op}[q\mathrm{e}^{\mathrm{i}sq}]\|_1\,\mathrm{d}s\right)|\hat{f}(t)|\,\mathrm{d}t,$$

where the notation $[0,t]$ is taken to mean $[t,0]$ when $t<0$.

Proof. Denote $A := \mathrm{op}[q]$, denote $U(t) := \mathrm{e}^{\mathrm{i}tA}$ as in Lemma 3.2.1, and denote $E(t) := \mathrm{op}[\mathrm{e}^{\mathrm{i}tq}]$ as in Lemma 3.2.2. We have

$$\tfrac{\mathrm{d}}{\mathrm{d}t}(E(t)U(-t)) = E'(t)U(-t)-\mathrm{i}E(t)AU(-t).$$

Integrating this on $[0,t]$ and applying the fundamental theorem of calculus (Theorem 3.1.9), we obtain

$$E(t)U(-t)-I_{L^2} = \int_0^t (E'(s)-\mathrm{i}E(s)A)U(-s)\,\mathrm{d}s,$$

so that

$$E(t)-U(t) = \int_0^t (E'(s)-\mathrm{i}E(s)A)U(-s)\,\mathrm{d}s\,U(t) =: R(t).$$

Multiplying by $\frac{1}{\sqrt{2\pi}}\hat{f}(t)$ and integrating we obtain

$$f(\mathrm{op}[q])-\mathrm{op}[f(q)] = \frac{1}{\sqrt{2\pi}}\int R(t)\hat{f}(t)\,\mathrm{d}t.$$

Applying Lemma 3.1.8 to $R(t)$ we obtain

$$\|R(t)\|_1 \leqslant \int_{[0,t]}\|E'(s)-\mathrm{i}E(s)A\|_1\|U(-s)\|\,\mathrm{d}s\|U(t)\| = \int_{[0,t]}\|E'(s)-\mathrm{i}E(s)A\|_1\,\mathrm{d}s,$$

and applying Lemma 3.1.8 again to the integral of $R(t)\hat{f}(t)$ we obtain the stated result. □

A consequence of the definition $f(A) := T^*f(a)T$ and the fact that $\|A\| = \|a\|_{L^\infty(M,\eta)}$ is that if

$$g(t) = f(t), \qquad \forall t : |t| \leqslant \|A\|,$$

then $f(A) = g(A)$. In particular, by using the lemma below we may use Lemma 3.2.3 with any smooth function.

Lemma 3.2.4. *Let $f \in C^\infty(\mathbb{R})$ and $H \in \mathbb{R}$ such that $H \geqslant 1$. Then there exists $g \in C_0^\infty(\mathbb{R})$ such that $f(t) = g(t)$ for $|t| \leqslant H$, and for each $S \geqslant 0$ there exists C_S (not dependent on f or t) such that*

$$|\hat{g}(t)| \leqslant C_S \frac{1}{\langle t\rangle^S}\sum_{j=0}^{S}\int_{-2H}^{2H}|f^{(j)}(y)|\,\mathrm{d}y.$$

Proof. Let $\zeta \in C_0^\infty(\mathbb{R})$ satisfy

$$\zeta(t) = \begin{cases} 1 & \text{when } |t| \leqslant 1, \\ 0 & \text{when } |t| \geqslant 2. \end{cases}$$

We set $g(t) := f(t)\zeta(t/H)$, so that $f(t) = g(t)$ for $|t| \leqslant H$. The Fourier transform of g satisfies

$$\hat{g}(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}ty} (P_{y,t}^{\mathrm{T}})^S g(y)\,\mathrm{d}y,$$

so applying Lemma 2.2.4 and collecting terms gives

$$|\hat{g}(t)| \leqslant C'_S \frac{1}{\langle t\rangle^S} \sum_{j=0}^{S} \int_{\mathbb{R}} |\partial^j (\zeta(y/H) f(y))|\,\mathrm{d}y.$$

Now applying the product rule and bounding $1/H \leqslant 1$ gives the stated result. □

3.3 Analytic functions of general operators

The construction of functions of operators described in §3.2 allows quite general functions but only applies when the operator is self adjoint. For operators that are not necessarily self adjoint we can still define polynomial functions of them by defining powers as iterated compositions. We can extend this to complex-analytic functions of operators by defining

$$f(A) := \lim_{N\to\infty} f_N(A), \qquad f_N(t) := \sum_{j=0}^{N} \frac{f^{(j)}(0)}{j!} t^j,$$

where the limit is taken in the operator norm topology. It is more usual to define complex-analytic functions of operators using Cauchy's integral formula, but the power series definition is simpler and sufficient for the purposes of this thesis, and allows us to briefly develop all of the facts needed.

We will use the notation $\operatorname{rad} f$ for the radius of convergence of f about 0. When A is a bounded operator and $\operatorname{rad} f > \|A\|$, for $M > N$ we have

$$\|f_M(A) - f_N(A)\| = \left\| \sum_{j=N+1}^{M} \frac{f^{(j)}(0)}{j!} A^j \right\| \leqslant \sum_{j=N+1}^{M} \frac{|f^{(j)}(0)|}{j!} \|A\|^j,$$

so f_N is a Cauchy sequence because $\sum_{j=0}^{\infty} f^{(j)}(0) z^j / j!$ is absolutely convergent when z is in the radius of convergence of f; this implies that the operator $f(A)$ exists (i.e. the sequence $f_N(A)$ converges in the norm topology) because the space of bounded operators is complete. The process of taking a function of an operator is linear in the function because, for $\alpha, \beta \in \mathbb{C}$,

$$\alpha f_N(A) + \beta g_N(A) = \alpha \sum_{j=0}^{N} \frac{f^{(j)}(0)}{j!} A^j + \beta \sum_{j=0}^{N} \frac{g^{(j)}(0)}{j!} A^j = \sum_{j=0}^{N} \frac{(\alpha f + \beta g)^{(j)}(0)}{j!} A^j = (\alpha f_N + \beta g_N)(A),$$

so if $\operatorname{rad} f > \|A\|$ and $\operatorname{rad} g > \|A\|$ then the limit of this equality says that

$$\alpha f(A) + \beta g(A) = (\alpha f + \beta g)(A).$$

We will be interested in functions of trace class operators. The basic properties of these are given in the next lemma.

Lemma 3.3.1. *Let A be a trace class operator (and therefore also a bounded operator) and f an analytic function with* $\operatorname{rad} f > \|A\|$ *(but not necessarily* $\operatorname{rad} f > \|A\|_1$*). Then the limit $f_N(A) \to f(A)$ converges in trace norm. If, further, $f(0) = 0$ then $f(A)$ is a trace class operator satisfying the finite bound*

$$\|f(A)\|_1 \leqslant \|A\|_1 \sum_{j=1}^{\infty} \frac{|f^{(j)}(0)|}{j!} \|A\|^{j-1}.$$

Proof. Denote $a_j := f^{(j)}(0)/j!$ for the coefficients of f. Assume that $A \neq 0$, otherwise the result is trivially true.

<u>$f_N(A) \to f(A)$ in trace norm.</u> Set $\tilde{f}(z) := f(z) - f(0)$ so that $\tilde{f}(0) = 0$, and in particular $\tilde{f}_N(A)$ is trace class for each $N \in \mathbb{N}_0$. For $M > N > 0$ we have

$$\|\tilde{f}_M(A) - \tilde{f}_N(A)\|_1 = \left\| \sum_{j=N+1}^{M} a_j A^j \right\|_1 \leqslant \sum_{j=N+1}^{M} |a_j| \, \|A\|_1 \, \|A\|^{j-1} = \frac{\|A\|_1}{\|A\|} \sum_{j=N+1}^{M} |a_j| \, \|A\|^j,$$

so $\tilde{f}_N$ is a Cauchy sequence in the trace norm topology because $\sum_{j=1}^{\infty} a_j z^j$ is absolutely convergent when z is in the radius of convergence of f. Each $\tilde{f}_N(A)$ is trace class and the space of trace class operators is complete (Birman and Solomjak, 1987, Theorem 11.2.6) so the sequence $\tilde{f}_N$ has a trace class limit, which equals $\tilde{f}$ because the trace norm limit is consistent with the operator norm limit. Finally, note that

$$f(A) = f(0)I + \tilde{f}(A), \quad f_N(A) = f(0)I + \tilde{f}_N(A),$$

so $\|f_N(A) - f(A)\|_1 = \|\tilde{f}_N(A) - \tilde{f}(A)\|_1 \to 0$ as $N \to \infty$. If $f(0) = 0$ then $\tilde{f} = f$ and so $f(A)$ is trace class.

<u>Trace norm of $f(A)$.</u> We now consider f satisfying $f(0) = 0$. For each $N \in \mathbb{N}_0$ we have

$$\|f_N(A)\|_1 = \left\| \sum_{j=1}^{N} a_j A^j \right\|_1 \leqslant \|A\|_1 \sum_{j=1}^{N} |a_j| \, \|A\|^{j-1} \leqslant \|A\|_1 \sum_{j=1}^{\infty} |a_j| \, \|A\|^{j-1} =: K.$$

This is finite because

$$K = \frac{\|A\|_1}{\|A\|} \sum_{j=1}^{\infty} |a_j| \, \|A\|^j,$$

and, again, $\sum_{j=1}^{\infty} a_j z^j$ is absolutely convergent when z is in the radius of convergence of f. We now show that $\|f(A)\|_1$ is bounded by K. Apply the reverse triangle inequality to obtain

$$\Big| \|f(A)\|_1 - \|f_N(A)\|_1 \Big| \leqslant \|f(A) - f_N(A)\|_1 \to 0,$$

so $\lim_{N\to\infty} \|f_N(A)\|_1 = \|f(A)\|_1$. We have shown that each $\|f_N(A)\|_1 \leqslant K$, so it follows that the limit is also bounded by K. $\square$

We will also need an analogue of first part of the above lemma for pseudodifferential operators with symbols of the form $f(q(\boldsymbol{z}))$.

Lemma 3.3.2. *Let $q \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ such that $q \in L^1(\mathbb{R}^{2d})$. Let f be an analytic function such that* $\operatorname{rad} f > \|q\|_{L^\infty(\mathbb{R}^{2d})}$. *Then* $\operatorname{op}[f_N(q)] \to \operatorname{op}[f(q)]$ *in trace norm.*

Proof. Assume that $q \not\equiv 0$ otherwise the result is trivial (because then $f_N(q) = f(q)$ for all $N \geqslant 0$).

Bound for derivatives of $g(q(\boldsymbol{z}))$. Let g be an analytic function with $\operatorname{rad} g > \|q\|_{L^\infty}$ and $g^{(n)}(0) = 0$ for each $n \leqslant K$ where $K \geqslant 0$. (Later, we will choose $g = f - f_N$.) By repeatedly applying the product and chain rule, for each multi-index $\boldsymbol{k} \in \mathbb{N}_0^{2d}$ such that $\boldsymbol{k} \neq \boldsymbol{0}$ and $|\boldsymbol{k}| \leqslant K$ we find that

$$\partial_{\boldsymbol{z}}^{\boldsymbol{k}}\big(g(q(\boldsymbol{z}))\big) = \sum_{n=1}^{|\boldsymbol{k}|} r_{n,\boldsymbol{k}}(\boldsymbol{z}) g^{(n)}(q(\boldsymbol{z})),$$

where each $r_{n,\boldsymbol{k}}(\boldsymbol{z})$ is a sum of products of n factors, each of which is of the form $\partial^{\boldsymbol{l}} q(\boldsymbol{z})$ with $\boldsymbol{l} \leqslant \boldsymbol{k}$ (which we bound by $\|\partial^{\boldsymbol{l}} q\|_{L^\infty}$). We will bound

$$|g^{(n)}(q(\boldsymbol{z}))| \leqslant \left| \sum_{j=1}^{\infty} a_j^{(n)} \big(q(\boldsymbol{z})\big)^j \right| \leqslant \frac{|q(\boldsymbol{z})|}{\|q\|_{L^\infty}} \sum_{j=1}^{\infty} |a_j^{(n)}| \, \|q\|_{L^\infty}^j,$$

where the $\{a_j^{(n)}\}$ are the coefficients for $g^{(n)}$ (which may be expressed in terms of $\{a_j^{(0)}\}$). A power series is absolutely convergent in its radius of convergence and satisfies $\operatorname{rad} g^{(n)} = \operatorname{rad} g$, so this bound is finite. We therefore have the finite bound

$$\left|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}\big(g(q(\boldsymbol{z}))\big)\right| \leqslant C_K |q(\boldsymbol{z})| \frac{\langle \|q\|_{L^\infty} \rangle^K}{\|q\|_{L^\infty}} \sum_{n=1}^{|\boldsymbol{k}|} \sum_{j=1}^{\infty} |a_j^{(n)}| \, \|q\|_{L^\infty}^j.$$

$\operatorname{op}[f_N(q)] \to \operatorname{op}[f(q)]$ in trace norm. By Lemma 2.1.3 we have

$$\|\operatorname{op}[f_N(q)] - \operatorname{op}[f(q)]\|_1 = \|\operatorname{op}[f_N(q) - f(q)]\|_1 \leqslant C_d \sum_{|\boldsymbol{k}| \leqslant 2d+1} \int_{\mathbb{R}^{2d}} \left|\partial_{\boldsymbol{z}}^{\boldsymbol{k}}\big(f_N(q(\boldsymbol{z})) - f(q(\boldsymbol{z}))\big)\right| \mathrm{d}\boldsymbol{z}.$$

For $N > n$ we have $f_N^{(n)}(0) - f(0) = 0$, so we apply the above bound with $K = 2d+1$ for $N > K$, giving

$$\|\operatorname{op}[f_N(q)] - \operatorname{op}[f(q)]\|_1 \leqslant C_d' \int_{\mathbb{R}^{2d}} |q(\boldsymbol{z})| \, \mathrm{d}\boldsymbol{z} \, \frac{\langle \|q\|_{L^\infty} \rangle^K}{\|q\|_{L^\infty}} \sum_{n=1}^{2d+1} \sum_{j=1}^{\infty} |a_{j;N}^{(n)}| \, \|q\|_{L^\infty}^j,$$

where $a_{j;N}^{(n)}$ is the j^{th} coefficient of $f - f_N$. The right hand side is finite because $q \in L^1(\mathbb{R}^{2d})$, and converges to zero as $N \to \infty$ because $a_{j;N}^{(n)} = 0$ for $N > j - n$. □

We are now ready to apply the above theory to pseudodifferential operators. This will be the only fact about analytic functions of operators needed to prove the main result of this thesis, except for the observation in Lemma 3.3.1 that if A is trace class and $f(0) = 0$ then $f(A)$ is trace class.

Lemma 3.3.3. *Let $q \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ such that $q \in L^1(\mathbb{R}^{2d})$ and* $\operatorname{op}[q]$ *is trace class. Let f be an analytic function such that* $\operatorname{rad} f = \infty$. *If there exist numbers $C_1, C_2, C_3 \geqslant 0$ such that for each*

$k \in \mathbb{N}$ we have

$$\|\mathrm{op}[q^{k+1}] - \mathrm{op}[q^k]\,\mathrm{op}[q]\|_1 \leqslant C_1 k^{C_2} C_3^k$$

then

$$\|f(\mathrm{op}[q]) - \mathrm{op}[f(q)]\|_1 \leqslant C_1 G(C_2, C_3, \|\mathrm{op}[q]\|; f),$$

where $G(C_2, C_3, \|\mathrm{op}[q]\|; f)$ is a finite quantity depending on its stated parameters (not on C_1). Furthermore, $G(a, b, c; f)$ is an increasing function of a, b and c.

Proof. We have

$$\begin{aligned}&\|f(\mathrm{op}[q]) - \mathrm{op}[f(q)]\|_1\\ &\qquad \leqslant \|f(\mathrm{op}[q]) - f_N(\mathrm{op}[q])\|_1 + \|f_N(\mathrm{op}[q]) - \mathrm{op}[f_N(q)]\|_1 + \|\mathrm{op}[f_N(q)] - \mathrm{op}[f(q)]\|_1.\end{aligned}$$

The first of these three terms converges to zero by Lemma 3.3.1 and the third converges to zero by Lemma 3.3.2. The second satisfies

$$\begin{aligned}\|f_N(\mathrm{op}[q]) - \mathrm{op}[f_N(q)]\|_1 &= \left\| \sum_{j=0}^{N} a_j\,\mathrm{op}[q]^j - \sum_{j=0}^{N} a_j\,\mathrm{op}[q^j] \right\|_1\\ &\leqslant \sum_{j=2}^{N} |a_j|\,\|\mathrm{op}[q]^j - \mathrm{op}[q^j]\|_1.\end{aligned}$$

But for $j \geqslant 2$ we have

$$\begin{aligned}\|\mathrm{op}[q]^j - \mathrm{op}[q^j]\|_1 &\leqslant \sum_{k=1}^{j-1} \|\mathrm{op}[q^{k+1}]\,\mathrm{op}[q]^{j-k-1} - \mathrm{op}[q^k]\,\mathrm{op}[q]^{j-k}\|_1\\ &\leqslant \sum_{k=1}^{j-1} \|\mathrm{op}[q]\|^{j-k-1} \|\mathrm{op}[q^{k+1}] - \mathrm{op}[q^k]\,\mathrm{op}[q]\|_1\\ &\leqslant C_1 \sum_{k=1}^{j-1} \|\mathrm{op}[q]\|^{j-k-1} k^{C_2} C_3^k\\ &\leqslant C_1 \sum_{k=1}^{j-1} (j-1)^{C_2} \big(\max\{C_3, \|\mathrm{op}[q]\|\}\big)^{j-1}\\ &= C_1 (j-1)^{C_2+1} \big(\max\{C_3, \|\mathrm{op}[q]\|\}\big)^{j-1}.\end{aligned}$$

By Bernoulli's inequality we have $j < 2^j$ so $(j-1)^{C_2+1} \leqslant (2^{C_2+1})^j$. Therefore, setting

$$K := \max\{2^{C_2+1} C_3, 2^{C_2+1} \|\mathrm{op}[q]\|, 1\},$$

we have

$$\|f_N(\mathrm{op}[q]) - \mathrm{op}[f_N(q)]\|_1 \leqslant C_1 \sum_{j=2}^{N} |a_j| K^j \leqslant C_1 \sum_{j=2}^{\infty} |a_j| K^j.$$

This is finite because K is within the radius of convergence of f. □

3.4 Trace norm bound for functions of pseudodifferential operators

In this section we put together the relevant pieces of the prior sections of this chapter with the trace norm bound for composition proved in §2.3.

To avoid repeatedly writing out the expression for the bound in Lemma 2.3.9 (which was stated in Lemma 2.3.5 and Remark 2.3.6), we will denote it $\mathsf{M}^{G,D}(F)$, as defined below.

Notation 3.4.1. Let $G, D \in \mathbb{N}_0$ and let $F \in C^D(\mathbb{R}^{4d})$. Then we denote

$$\mathsf{M}^{G,D}(F) := \sum_{\substack{\boldsymbol{m}\in\mathbb{N}_0^{4d}\\ |\boldsymbol{m}|\leqslant D}} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{|\partial^{\boldsymbol{m}} F(\boldsymbol{x},\boldsymbol{y})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^G} \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}.$$

In particular, this is symmetric i.e. $\mathsf{M}^{G,D}(F(\boldsymbol{x},\boldsymbol{y})) = \mathsf{M}^{G,D}(F(\boldsymbol{y},\boldsymbol{x}))$, and sublinear i.e. for $\lambda > 0$ and $F_1, F_2 \in C^D(\mathbb{R}^{4d})$ we have

$$\mathsf{M}^{G,D}(\lambda F) = \lambda \mathsf{M}^{G,D}(F), \qquad \mathsf{M}^{G,D}(F_1 + F_2) \leqslant \mathsf{M}^{G,D}(F_1) + \mathsf{M}^{G,D}(F_2).$$

It will be helpful when manipulating these expressions to use Sobolev norms (with a positive integer number of derivatives), which for $1 \leqslant p \leqslant \infty$ and $a \in C^D(\mathbb{R}^{2d})$ are defined as

$$\mathsf{N}_p^D(a) := \sum_{|\boldsymbol{m}|\leqslant D} \|\partial^{\boldsymbol{m}} a\|_{L^p(\mathbb{R}^{2d})}.$$

In particular, $\|\mathrm{op}[q]\| \leqslant C_d \mathsf{N}_\infty^{d+2}(q)$ and $\|\mathrm{op}[q]\|_1 \leqslant C_d' \mathsf{N}_1^{2d+1}(q)$.

Lemma 3.4.2. *Let $G, D \in \mathbb{N}_0$, $a, b \in C^D(\mathbb{R}^{2d})$ and $F \in C^D(\mathbb{R}^{4d})$. Then*

$$\mathsf{M}^{G,D}(a(\boldsymbol{x})F(\boldsymbol{x},\boldsymbol{y})) \leqslant C_D \mathsf{N}_\infty^D(a) \mathsf{M}^{G,D}(F), \qquad \mathsf{M}^{G,D}(a(\boldsymbol{x})b(\boldsymbol{y})) \leqslant C_D I_G \mathsf{N}_\infty^D(a) \mathsf{N}_1^D(b),$$

where $I_G := \int_{\mathbb{R}^{2d}} \langle \boldsymbol{v}\rangle^{-G}\,\mathrm{d}\boldsymbol{v}$, which is finite when $G > 2d$.

Proof. First inequality. By the product rule we have, for $\boldsymbol{k}_1, \boldsymbol{k}_2 \in \mathbb{N}_0^{2d}$,

$$\partial_{\boldsymbol{x}}^{\boldsymbol{k}_1} \partial_{\boldsymbol{y}}^{\boldsymbol{k}_2} \Big(a(\boldsymbol{x}) F(\boldsymbol{x},\boldsymbol{y}) \Big) = \sum_{\boldsymbol{l}\leqslant \boldsymbol{k}_1} \binom{\boldsymbol{k}_1}{\boldsymbol{l}} \partial^{\boldsymbol{k}_1-\boldsymbol{l}} a(\boldsymbol{x}) \partial_{\boldsymbol{x}}^{\boldsymbol{l}} \partial_{\boldsymbol{y}}^{\boldsymbol{k}_2} F(\boldsymbol{x},\boldsymbol{y}).$$

Thus, when $|\boldsymbol{k}_1| + |\boldsymbol{k}_2| \leqslant D$, we have

$$\begin{aligned} \Big| \partial_{\boldsymbol{x}}^{\boldsymbol{k}_1} \partial_{\boldsymbol{y}}^{\boldsymbol{k}_2} \Big(a(\boldsymbol{x}) F(\boldsymbol{x},\boldsymbol{y}) \Big) \Big| &\leqslant \sum_{\boldsymbol{l}\leqslant \boldsymbol{k}_1} \binom{\boldsymbol{k}_1}{\boldsymbol{l}} |\partial^{\boldsymbol{k}_1-\boldsymbol{l}} a(\boldsymbol{x})| |\partial_{\boldsymbol{x}}^{\boldsymbol{l}} \partial_{\boldsymbol{y}}^{\boldsymbol{k}_2} F(\boldsymbol{x},\boldsymbol{y})| \\ &\leqslant \mathsf{N}_\infty^D(a) \Bigg(\sum_{|\boldsymbol{m}|\leqslant D} |\partial^{\boldsymbol{m}} F(\boldsymbol{x},\boldsymbol{y})| \Bigg) \sum_{\boldsymbol{l}\leqslant \boldsymbol{k}_1} \binom{\boldsymbol{k}_1}{\boldsymbol{l}}. \end{aligned}$$

Summing over $\boldsymbol{k}_1, \boldsymbol{k}_2$ gives the result, with

$$C_D = \sum_{|\boldsymbol{k}_1|+|\boldsymbol{k}_2|\leqslant D} \sum_{\boldsymbol{l}\leqslant \boldsymbol{k}_1} \binom{\boldsymbol{k}_1}{\boldsymbol{l}}.$$

Second inequality. By the first inequality we have

$$\mathsf{M}^{G,D}(a(\boldsymbol{x})b(\boldsymbol{y})) \leqslant C_D \mathsf{N}^D_\infty(a)\mathsf{M}^{G,D}(b(\boldsymbol{y})).$$

But, changing variables $\boldsymbol{v} := \boldsymbol{x}-\boldsymbol{y}$ in the d$\boldsymbol{x}$ integral,

$$\begin{aligned}\mathsf{M}^{G,D}(b(\boldsymbol{y})) &= \sum_{|\boldsymbol{m}_1|+|\boldsymbol{m}_2|\leqslant D} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{|\partial_{\boldsymbol{x}}^{\boldsymbol{m}_1}\partial_{\boldsymbol{y}}^{\boldsymbol{m}_2} b(\boldsymbol{y})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^G}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\\ &= \sum_{|\boldsymbol{m}_2|\leqslant D} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{|\partial_{\boldsymbol{y}}^{\boldsymbol{m}_2} b(\boldsymbol{y})|}{\langle \boldsymbol{x}-\boldsymbol{y}\rangle^G}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}\\ &= \sum_{|\boldsymbol{m}_2|\leqslant D} \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{|\partial_{\boldsymbol{y}}^{\boldsymbol{m}_2} b(\boldsymbol{y})|}{\langle \boldsymbol{v}\rangle^G}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{y} = I_G \mathsf{N}^D_1(b). \qquad\square\end{aligned}$$

We now prove the main result of this section: the trace norm bound for the difference of $f(\mathrm{op}[q])$ and $\mathrm{op}[f(q)]$.

Lemma 3.4.3. *Let $q \in C^\infty_{\mathrm{b}}(\mathbb{R}^{2d})$ such that $\partial^{\boldsymbol{k}} q \in L^1(\mathbb{R}^{2d})$ for each $\boldsymbol{k} \in \mathbb{N}^{2d}_0$. Let either one of the following be satisfied:*

- *The function $f \in C^\infty(\mathbb{R})$ and q is real-valued.*
- *The function f is complex analytic on $\mathbb{C}$ (i.e. has infinite radius of convergence).*

Let $G > 2d$ and set $D := G + 4d + 2$. Then

$$\|\mathrm{op}[f(q)] - f(\mathrm{op}[q])\|_1 \leqslant K(\mathsf{N}^D_\infty(q), f, d, G)\,\mathsf{M}^{G,D}(F_1),$$

where

$$F_1(\boldsymbol{x},\boldsymbol{y}) := \frac{\mathrm{i}}{2}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})(q(\boldsymbol{x})q(\boldsymbol{y})),$$

and where $K(\mathsf{N}^D_\infty(q), f, d, G)$ is a finite constant depending on its stated parameters but not otherwise depending on q; furthermore, $K(a, f, d, G)$ is an increasing function of a for $a \geqslant 0$.

Proof. Self-adjoint case. We make use of Lemma 3.2.4 with $H = \langle \max\{\|q\|_{L^\infty}, \|\mathrm{op}[q]\|\}\rangle$ and $S = D + 4$ to choose $g \in C^\infty_0(\mathbb{R})$; in particular, $g(\mathrm{op}[q]) = f(\mathrm{op}[q])$ and $\mathrm{op}[f(q)] = \mathrm{op}[g(q)]$. Applying Lemma 3.2.3 and then Lemma 2.3.9 (since $\mathrm{e}^{\mathrm{i}sq} \in C^\infty_{\mathrm{b}}(\mathbb{R}^{2d})$ for each $s \in \mathbb{R}$), we have

$$\begin{aligned}\|f(\mathrm{op}[q]) - \mathrm{op}[f(q)]\|_1 &= \|g(\mathrm{op}[q]) - \mathrm{op}[g(q)]\|_1\\ &\leqslant \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\left(\int_{[0,t]} \|\mathrm{op}[\mathrm{e}^{\mathrm{i}sq}]\mathrm{op}[q] - \mathrm{op}[q\mathrm{e}^{\mathrm{i}sq}]\|_1\,\mathrm{d}s\right)|\hat{g}(t)|\,\mathrm{d}t\\ &\leqslant \frac{1}{\sqrt{2\pi}} C_{d,G}\int_{\mathbb{R}}\left(\int_{[0,t]} \mathsf{M}^{G,D}(\widetilde{F}_1(\boldsymbol{x},\boldsymbol{y};s))\,\mathrm{d}s\right)|\hat{g}(t)|\,\mathrm{d}t,\end{aligned}$$

where

$$\begin{aligned}\widetilde{F}_1(\boldsymbol{x},\boldsymbol{y};s) &= \frac{\mathrm{i}}{2}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})(q(\boldsymbol{x})\mathrm{e}^{\mathrm{i}sq(\boldsymbol{y})})\\ &= \frac{\mathrm{i}^2}{2} s\,\mathrm{e}^{\mathrm{i}sq(\boldsymbol{y})}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})(q(\boldsymbol{x})q(\boldsymbol{y})).\end{aligned}$$

By Lemma 3.4.2 we thus have

$$\mathsf{M}^{G,D}(\widetilde{F}_1(\boldsymbol{x},\boldsymbol{y};s)) \leqslant C_D s \mathsf{N}_\infty^D(\mathrm{e}^{\mathrm{i}sq(\boldsymbol{y})})\mathsf{M}^{G,D}(F_1).$$

But we may find the derivatives of $\mathrm{e}^{\mathrm{i}sq(\boldsymbol{y})}$ as in the proof Lemma 3.2.2 (with $l=n=0$), giving

$$\mathsf{N}_\infty^D(\mathrm{e}^{\mathrm{i}sq(\boldsymbol{y})}) \leqslant \sum_{|\boldsymbol{k}|\leqslant D} \sup_{\boldsymbol{z}\in\mathbb{R}^{2d}} \sum_{j=0}^{|\boldsymbol{k}|} |s|^j |r_{j,\boldsymbol{k},0,0}(\boldsymbol{z})| \leqslant C_D' \langle s\rangle^D \Big\langle \mathsf{N}_\infty^D(q)\Big\rangle^D.$$

Combining the above, we find that

$$\|f(\mathrm{op}[q]) - \mathrm{op}[f(q)]\|_1 \leqslant \frac{1}{\sqrt{2\pi}} C_{d,G} C_D C_D' \int_{\mathbb{R}} \bigg(\int_{[0,t]} \langle s\rangle^{D+1}\,\mathrm{d}s\bigg)|\hat{g}(t)|\,\mathrm{d}t \Big\langle \mathsf{N}_\infty^D(q)\Big\rangle^D \mathsf{M}^{G,D}(F_1).$$

The $\mathrm{d}s$ integral is a constant multiple of $\langle t\rangle^{D+2}$, so the $\mathrm{d}t$ integral is bounded by a multiple of

$$\int_{\mathbb{R}} \frac{\langle t\rangle^{D+2}}{\langle t\rangle^{D+4}}\,\mathrm{d}t \sum_{j=0}^{D+4} \int_{-2\langle\|\mathrm{op}[q]\|\rangle}^{2\langle\|\mathrm{op}[q]\|\rangle} |f^{(j)}(y)|\,\mathrm{d}y.$$

But $1/\langle t\rangle^2$ is integrable, so bounding $\|\mathrm{op}[q]\| \leqslant C_d \mathsf{N}_\infty^{d+2}(q) \leqslant C_d \mathsf{N}_\infty^D(q)$ completes the proof.

Analytic function case. For each $k\in\mathbb{N}$, by Lemma 2.3.9 we have

$$\|\mathrm{op}[q^{k+1}] - \mathrm{op}[q^k]\,\mathrm{op}[q]\|_1 \leqslant C_{d,G} \mathsf{M}^{G,D}(\widetilde{F}_1),$$

where

$$\begin{aligned}
\widetilde{F}_1(\boldsymbol{x},\boldsymbol{y}) &= \frac{\mathrm{i}}{2}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})\big((q(\boldsymbol{x}))^k q(\boldsymbol{y})\big)\\
&= \frac{\mathrm{i}}{2} k (q(\boldsymbol{x}))^{k-1}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})(q(\boldsymbol{x})q(\boldsymbol{y})).
\end{aligned}$$

By Lemma 3.4.2 we have

$$\mathsf{M}^{G,D}(\widetilde{F}_1) \leqslant C_D k \mathsf{N}_\infty^D(q^{k-1})\mathsf{M}^{G,D}(F_1).$$

Considering the function q^{k-1} as the product of $k-1$ factors, we see that a partial derivative of it is the sum of terms that are again each the product of $k-1$ factors. Continuing inductively, we find that for $\boldsymbol{m}\leqslant D$ we have

$$|\partial^{\boldsymbol{m}}(q(\boldsymbol{z}))^{k-1}| \leqslant (k-1)^{|\boldsymbol{m}|}\Big(\max_{\boldsymbol{n}\leqslant\boldsymbol{m}} |\partial^{\boldsymbol{n}} q(\boldsymbol{z})|\Big)^{k-1} \leqslant (k-1)^D \Big(\mathsf{N}_\infty^D(q)\Big)^{k-1},$$

so

$$\mathsf{N}_\infty^D(q^{k-1}) \leqslant \sum_{|\boldsymbol{m}|\leqslant D} (k-1)^D \Big(\mathsf{N}_\infty^D(q)\Big)^{k-1} = (2d)^D (k-1)^D \Big(\mathsf{N}_\infty^D(q)\Big)^{k-1}.$$

Combining the above, we therefore have

$$\|\mathrm{op}[q^{k+1}] - \mathrm{op}[q^k]\,\mathrm{op}[q]\|_1 \leqslant C_{d,G} C_D (2d)^D k^{D+1} \langle \mathsf{N}_\infty^D(q)\rangle^k \mathsf{M}^{G,D}(F_1).$$

The result now follows by applying Lemma 3.3.3 and bounding $\|\mathrm{op}[q]\| \leqslant \mathsf{N}_\infty^{d+2}(q) \leqslant \mathsf{N}_\infty^D(q)$. $\square$

Chapter 4

Tubular neighbourhood theory

A tubular neighbourhood of a smooth manifold $\mathit{\Gamma} \subseteq \mathbb{R}^m$ is a set of points near to $\mathit{\Gamma}$ that, roughly speaking, does not intersect itself. (A precise definition is given in §4.2.) For example, if $\mathit{\Gamma}$ is a closed curve in $\mathbb{R}^3$ then a tubular neighbourhood is literally a tube in the intuitive sense (including the points inside the tube — not just a tubular shell), requiring that the tube's radius is not greater than the curve's radius of curvature nor greater than the closest the curve gets to itself (as in the neck of an hourglass-shaped curve).

The seminal work on tubes was the paper by Weyl (1939), which contained a formula for the volume of these tubes as a function of the tubular radius. He proved this by first showing the change of variables formula

$$\int_{\mathrm{tub}_t(\mathit{\Gamma})} f(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = \int_{\mathit{\Gamma}} \int_{N_t^{\boldsymbol{u}}} f(\boldsymbol{u}+\boldsymbol{n}) \det(I - S^{\boldsymbol{u}}(\boldsymbol{n}))\,\mathrm{d}\boldsymbol{n}\,\mathrm{d}\boldsymbol{u},$$

where $N_t^{\boldsymbol{u}}$ is a subset of the normal space at $\boldsymbol{u}$ and $S^{\boldsymbol{u}}(\boldsymbol{n})$ is a matrix depending on the curvature of $\mathit{\Gamma}$. Substituting $f \equiv 1$ gives the volume of the tube, and it remains to evaluate the integral of the Jacobian.

Tubular theory will be useful for us because we will have to manipulate (especially integrate) functions whose value is concentrated within a constant distance of $r\mathit{\Gamma}$, where r is a large scaling parameter and $\mathit{\Gamma} \subseteq \mathbb{R}^m$ is a sufficiently smooth k-dimensional manifold. (Viewed from another perspective, such functions are concentrated within a small distance $1/r$ of a constant-sized region $\mathit{\Gamma}$.) For example, we will need to bound

$$I := \int_{\mathrm{tub}_{rt}(r\mathit{\Gamma})} b\big(\mathrm{near}(\boldsymbol{z}, r\mathit{\Gamma})/r\big)\psi\big(\mathrm{dist}(\boldsymbol{z}, r\mathit{\Gamma})\big)\,\mathrm{d}\boldsymbol{z},$$

where $\mathrm{near}(\boldsymbol{z},\mathit{\Gamma})$ denotes the nearest point on $\mathit{\Gamma}$ to $\boldsymbol{z}$ and $\mathrm{dist}(\boldsymbol{z},\mathit{\Gamma})$ denotes the distance from $\boldsymbol{z}$ to $\mathrm{near}(\boldsymbol{z},\mathit{\Gamma})$. Here r is a large scaling parameter, so if $\mathit{\Gamma}$ is compact then, bounding b and ψ by their maxima, we can bound I by a multiple of the volume of the tube $\mathrm{tub}_{rt}(r\mathit{\Gamma})$, which is proportional to r^m. But using the above change of variables we obtain the improved bound

$$|I| \leqslant M \int_{r\mathit{\Gamma}} \int_{N_{rt}^{\boldsymbol{u}}} b(\boldsymbol{u}/r)\psi(|\boldsymbol{n}|)\,\mathrm{d}\boldsymbol{n}\,\mathrm{d}\boldsymbol{u} \propto r^k \|b\|_{L^1(\mathit{\Gamma})} \|\psi\|_{L^1(\mathbb{R}_+)}.$$

The most basic results in this chapter are of this form: within a distance proportional to r we obtain a uniform bound. But our most critical results are bounds that hold more precisely when very close to Γ. For example, in addition to showing that the Jacobian does not get arbitrarily large i.e. using a bound of the form

$$|\det(I - S^{\boldsymbol{u}}(\boldsymbol{n}))| \leqslant M,$$

we will also show that, close to Γ, the Jacobian is approximately equal to 1 i.e. use a bound of the form

$$\left|\det(I - S^{\boldsymbol{u}}(\boldsymbol{n})) - 1\right| \leqslant \frac{L|\boldsymbol{n}|}{r}.$$

By now, the theory of tubular neighbourhoods is standard. However, in this chapter we develop the necessary theory in full, for two reasons. The first reason is that, to the author's knowledge, no systematic treatment has been published for the circumstances needed here. Differential geometry sources, such as the short book by Gray (2004), typically assume a more general ambient manifold than Euclidean space as required here but prove weaker results, usually requiring the embedded manifold to be bounded and C^∞ smooth. The treatment in the situation closest to here is the book by Gilbarg and Trudinger (1977, Appendix; moved to §14.6 in 1983 second edition), which is the inspiration for the approach of this chapter, but assumes the embedded manifold is codimension 1, while we will need codimension 2 for the "corners" of non-smooth domains. The second reason the theory is developed in full here is that we develop some very simple novel theory: rather than demanding that the manifolds involved are closed, we demand that they are "extensible", which requires that they are a subset of a slightly larger manifold. By proving the standard results first we are able to focus on the truly novel parts while developing this additional theory.

The chapter proceeds as follows. In §4.2 we define tubular neighbourhoods and establish their basic properties. In §4.3 we discuss curvature, including the change of variables formula discussed above. §4.4 contains a brief overview of further standard developments of the theory that are not covered in this chapter. In §4.5 we develop the notion of extensibility mentioned above. Finally, in §4.6 we crystallise out basic consequences of the theory that will be of use when proving the Szegő theorem.

4.1 Graph representations of manifolds in Euclidean space

In this section we fix some notations and conventions by defining the graph representations of manifolds embedded in Euclidean space and expressing the tangent and normal spaces in terms of these representations. Throughout this section we let $r \in \mathbb{N}_0$, representing the regularity of a manifold, and $k \in \mathbb{N}_0$, representing the dimension of the manifold (embedded in $\mathbb{R}^m$). We will define manifolds in terms of graph coordinates as follows.

Definition 4.1.1. We say that a set $\Gamma \subseteq \mathbb{R}^m$ is a C^r (respectively, Lipschitz) graph of dimension k at a point $\boldsymbol{u} \in \Gamma$ if there exists a neighbourhood $G^{\boldsymbol{u}}$ of $\boldsymbol{u}$ and a C^r (respectively, Lipschitz) function

$$g^{\boldsymbol{u}} : \mathbb{R}^k \to \mathbb{R}^{m-k}$$

such that (after rotating Γ) for any $\boldsymbol{z} \in G^{\boldsymbol{u}}$, writing $\boldsymbol{z} = (\boldsymbol{z}', \boldsymbol{z}'')$ with $\boldsymbol{z}' \in \mathbb{R}^k$ and $\boldsymbol{z}'' \in \mathbb{R}^{m-k}$, we have

$$\boldsymbol{z} \in \Gamma \quad \Longleftrightarrow \quad \boldsymbol{z}'' = g^{\boldsymbol{u}}(\boldsymbol{z}').$$

Remark 4.1.2. Regularity is often defined in terms of coordinate charts instead of graph representations. If a set is a C^r (resp. Lipschitz) graph at a point $\boldsymbol{u} \in \Gamma$ then it satisfies the chart condition because $\boldsymbol{z} \mapsto \boldsymbol{z}'' - g^{\boldsymbol{u}}(\boldsymbol{z}')$ is a coordinate chart (from Γ to $\mathbb{R}^k$) in a neighbourhood of $\boldsymbol{u}$. Conversely if a set is described by C^r chart in a neighbourhood of a point where $r \geqslant 1$ then a corresponding graph exists by the implicit function theorem. However, this converse does not hold for C^0 and Lipschitz charts; for this reason sets satisfying the Lipschitz graph condition are sometimes called *strongly Lipschitz*.

Definition 4.1.3. We say that a set $\Omega \subseteq \mathbb{R}^m$ is a C^r (resp. Lipschitz) epigraph at a point $\boldsymbol{u} \in \partial\Omega$ if there exists a neighbourhood $G^{\boldsymbol{u}}$ of $\boldsymbol{u}$ and a C^r (resp. Lipschitz) function

$$g^{\boldsymbol{u}} : \mathbb{R}^{m-1} \to \mathbb{R}$$

such that (after rotating Ω) for any $\boldsymbol{z} \in G^{\boldsymbol{u}}$, writing $\boldsymbol{z} = (\boldsymbol{z}', z'')$ with $\boldsymbol{z}' \in \mathbb{R}^{m-1}$ and $z'' \in \mathbb{R}$, we have

$$\begin{aligned} \boldsymbol{z} \in \Omega \setminus \partial\Omega \quad &\Longleftrightarrow \quad z'' > g^{\boldsymbol{u}}(\boldsymbol{z}'), \\ \boldsymbol{z} \in \partial\Omega \quad &\Longleftrightarrow \quad z'' = g^{\boldsymbol{u}}(\boldsymbol{z}'), \\ \boldsymbol{z} \in \Omega^{\mathrm{c}} \setminus \partial\Omega \quad &\Longleftrightarrow \quad z'' < g^{\boldsymbol{u}}(\boldsymbol{z}'). \end{aligned}$$

Clearly if Ω is a C^r (resp. Lipschitz) epigraph at a point then $\partial\Omega$ is a C^r (resp. Lipschitz) graph of dimension $m-1$ at that point. The converse does not hold; a counterexample is the whole space $\mathbb{R}^m$ with a hyperplane removed.

Definition 4.1.4. We say that a set $\Gamma \subseteq \mathbb{R}^m$ is a C^r (resp. Lipschitz) manifold of dimension k if it is a C^r (resp. Lipschitz) graph at every point. (For $k = 0$, we say it is a manifold if it is an isolated set of points in $\mathbb{R}^m$, and for $k = m$ we say it is a manifold if it is an open set in $\mathbb{R}^m$.) Similarly, we say that a set $\Omega \subseteq \mathbb{R}^m$ is a C^r (resp. Lipschitz) domain if it is a C^r (resp. Lipschitz) epigraph at every point in $\partial\Omega$.

For both the definition of manifolds and the definition of domains, there is no requirement that the $g^{\boldsymbol{u}}$, $G^{\boldsymbol{u}}$ or rotation at each point is the same as at any other point. However, for manifolds we do demand that every point is a graph of some fixed dimension k.

We do not demand that manifolds are closed sets by definition, so this says nothing about the regularity of the boundary (in the manifold sense) of $\varGamma$. For example, the unit square without edges or vertices embedded in $\mathbb{R}^3$ is a C^∞ manifold of dimension 2 under this definition, even though its manifold boundary is not even C^1. This terminology is consistent with Federer (1969, 3.1.19), for example. However, the case where the manifold is a closed set of particular interest, as we shall see in §4.2 and §4.5. Unlike the differential geometry literature, we will only ever used "closed" in the topological sense; there is no suggestion of boundedness unless specified.

We now turn our attention to the tangent space and normal space, which are used heavily in the study of tubular neighbourhoods.

Notation 4.1.5. Let $\varGamma \subseteq \mathbb{R}^m$ be a C^1 graph of dimension k at a point $\boldsymbol{u} \in \varGamma$. We denote the tangent space and normal space at that point by $T^{\boldsymbol{u}}(\varGamma)$ and $N^{\boldsymbol{u}}(\varGamma)$ respectively (see e.g. Federer, 1969, 3.1.21). These are orthogonal subspaces of $\mathbb{R}^m$ of dimension k and $m-k$ respectively (in particular they both contain the zero vector). Where there is no possibility of confusion we write simply $T^{\boldsymbol{u}}$ and $N^{\boldsymbol{u}}$.

Remark 4.1.6. A key property of $N^{\boldsymbol{u}}$ is that if $\boldsymbol{z} \in \mathbb{R}^m$ and $\boldsymbol{u} \in \varGamma$ such that $\operatorname{dist}(\boldsymbol{z}, \varGamma) = |\boldsymbol{z}-\boldsymbol{u}|$ (such a $\boldsymbol{u}$ is called a *nearest point* of $\boldsymbol{z}$ to $\varGamma$) and $\varGamma$ is a C^1 graph at $\boldsymbol{u}$ then $\boldsymbol{z}-\boldsymbol{u} \in N^{\boldsymbol{u}}$. This is shown, for example, in Federer (1959, Theorem 4.8(2)).

Notation 4.1.7. For any C^1 function $f\colon \mathbb{R}^n \to \mathbb{R}^m$, we define the Jacobian matrix to be the $m \times n$ matrix

$$\nabla \otimes f := \begin{pmatrix} \partial_1 f_1 & \cdots & \partial_n f_1 \\ \vdots & \ddots & \vdots \\ \partial_1 f_m & \cdots & \partial_n f_m \end{pmatrix}.$$

(The motivation for this notation is the usual outer product for vectors, although considering ∇ formally as a column vector of partial derivatives and f as a column vector, this is the transpose of the usual outer product i.e. with the above definition, $\nabla \otimes f := (\nabla f^{\mathrm{T}})^{\mathrm{T}}$.)

Remark 4.1.8. One use of tangent and normal spaces is to give a canonical way of expressing the graph representation of a manifold about a point. Let $\varGamma \subseteq \mathbb{R}^m$ be a C^r manifold with $r \geqslant 1$. For each point $\boldsymbol{u} \in \varGamma$ there is a neighbourhood $G^{\boldsymbol{u}} \subseteq \mathbb{R}^m$ and a C^r function

$$\omega^{\boldsymbol{u}}\colon T^{\boldsymbol{u}} \cap (-\boldsymbol{u} + G^{\boldsymbol{u}}) \to N^{\boldsymbol{u}}$$

such that for all $\boldsymbol{z} \in G^{\boldsymbol{u}}$ we have

$$\boldsymbol{z} \in \varGamma \quad \iff \quad \operatorname{proj}_{N^{\boldsymbol{u}}}(\boldsymbol{z}-\boldsymbol{u}) = \omega^{\boldsymbol{u}}(\operatorname{proj}_{T^{\boldsymbol{u}}}(\boldsymbol{z}-\boldsymbol{u})).$$

That is, for all $\boldsymbol{z} \in G^{\boldsymbol{u}}$, writing $\boldsymbol{z} = \boldsymbol{u} + \boldsymbol{t} + \boldsymbol{n}$ where $\boldsymbol{t} \in T^{\boldsymbol{u}}$ and $\boldsymbol{n} \in N^{\boldsymbol{u}}$, the condition on $\omega^{\boldsymbol{u}}$ is

$$\boldsymbol{z} \in \varGamma \quad \iff \quad \boldsymbol{n} = \omega^{\boldsymbol{u}}(\boldsymbol{t}).$$

When necessary we will rotate the coordinates so that $T^{\boldsymbol{u}} = \mathbb{R}^k \times \{\boldsymbol{0}_{m-k}\}$ and $N^{\boldsymbol{u}} = \{\boldsymbol{0}_k\} \times \mathbb{R}^{m-k}$, so that

$$\omega^{\boldsymbol{u}} : \mathbb{R}^k \cap (-\boldsymbol{v} + G^{\boldsymbol{u}}) \to \mathbb{R}^{m-k},$$

which for example allows us to make sense of $\nabla \otimes \omega^{\boldsymbol{u}}(\boldsymbol{t})$ as an $(m-k) \times k$ matrix. Such an $\omega^{\boldsymbol{u}}$ satisfies $\omega^{\boldsymbol{u}}(\boldsymbol{0}) = \boldsymbol{0}$, and $\nabla \otimes \omega^{\boldsymbol{u}}(\boldsymbol{0})$ is the zero matrix. From now on we always use $\omega^{\boldsymbol{u}}$ (and $G^{\boldsymbol{u}}$) to denote such a function.

One use of such graph representations is to write the tangent space and normal space of each point $\boldsymbol{v} \in \Gamma$ <u>near to</u> a point $\boldsymbol{u} \in \Gamma$ in terms of the tangent space and normal space <u>at</u> $\boldsymbol{u} \in \Gamma$.

Lemma 4.1.9. *Let $\Gamma \subseteq \mathbb{R}^m$ be C^1 manifold and let $\boldsymbol{u} \in \Gamma$. Then for each $\boldsymbol{v} \in \Gamma \cap G^{\boldsymbol{u}}$, writing $\boldsymbol{t} := \operatorname{proj}_{T^{\boldsymbol{u}}}(\boldsymbol{v} - \boldsymbol{u})$, we have*

$$T^{\boldsymbol{v}} = \{\boldsymbol{s} + (\boldsymbol{s} \cdot \nabla_{\boldsymbol{t}})\omega^{\boldsymbol{u}}(\boldsymbol{t}) \in \mathbb{R}^m : \boldsymbol{s} \in T^{\boldsymbol{u}}\},$$
$$N^{\boldsymbol{v}} = \{\boldsymbol{n} - \nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}})(\boldsymbol{t}) \in \mathbb{R}^m : \boldsymbol{n} \in N^{\boldsymbol{u}}\}.$$

This is a standard fact, and can be expressed in a variety of different ways. For example, the first expression is the pushforward of a coordinate chart, and the second can be thought of as a higher-codimension generalisation of the elementary fact that the gradient of a scalar-valued function is orthogonal to its level sets. Here is a simple coordinate-based proof.

Proof. For the expression for $T^{\boldsymbol{v}}$, note that $f(\boldsymbol{t}, \boldsymbol{n}) := \boldsymbol{u} + \boldsymbol{t} + \omega^{\boldsymbol{u}}(\boldsymbol{t}) + \boldsymbol{n}$ is map from $G^{\boldsymbol{u}} \subseteq \mathbb{R}^m$ to $\mathbb{R}^m$ that maps $T^{\boldsymbol{u}}$ to Γ, so $\nabla_{\boldsymbol{t}} \otimes f(\boldsymbol{t}, \boldsymbol{0})$ transforms $T^{\boldsymbol{u}}$ to $T^{\boldsymbol{v}}$ (see Federer, 1969, 3.1.21, top of p. 234). To see why the equality for $N^{\boldsymbol{v}}$ holds, first note that if $\boldsymbol{s} \in T^{\boldsymbol{u}}$ and $\boldsymbol{n} \in N^{\boldsymbol{u}}$ then

$$\begin{aligned} \boldsymbol{s} &\in T^{\boldsymbol{u}}, & (\boldsymbol{s} \cdot \nabla_{\boldsymbol{t}})\omega^{\boldsymbol{u}}(\boldsymbol{t}) &\in N^{\boldsymbol{u}}, \\ \boldsymbol{n} &\in N^{\boldsymbol{u}}, & -\nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}})(\boldsymbol{t}) &\in T^{\boldsymbol{u}}, \end{aligned}$$

and therefore

$$(\boldsymbol{s} + (\boldsymbol{s} \cdot \nabla_{\boldsymbol{t}})\omega^{\boldsymbol{u}}(\boldsymbol{t})) \cdot (\boldsymbol{n} - \nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}})(\boldsymbol{t})) = -\boldsymbol{s} \cdot \nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}})(\boldsymbol{t}) + (\boldsymbol{s} \cdot \nabla_{\boldsymbol{t}})\omega^{\boldsymbol{u}}(\boldsymbol{t}) \cdot \boldsymbol{n} = 0.$$

The stated expression is therefore contained in $N^{\boldsymbol{u}}$; but it has the same dimension as $N^{\boldsymbol{u}}$, so is indeed equal to $N^{\boldsymbol{u}}$. □

Remark 4.1.10. When applying Remark 4.1.8 to the boundary of a domain, as in Definition 4.1.3 we choose the rotation so that $\boldsymbol{z} \in \Omega$ when $n > \omega^{\boldsymbol{u}}(\boldsymbol{t})$ and $\boldsymbol{z} \in \Omega^{\mathrm{c}}$ when $n < \omega^{\boldsymbol{u}}(\boldsymbol{t})$. The corresponding normals expressed in Lemma 4.1.9 then lie on the same side of the boundary.

4.2 Tubular neighbourhoods

In this section we define what a tubular neighbourhood is and recall some basic properties that they possess. We then prove the tubular neighbourhood theorem, which is the fact that a C^2 manifold that is closed and bounded has a tubular neighbourhood.

We will start by defining some notation used in this chapter and, in the case of $B_t(\Gamma)$ and $\operatorname{tub}_t(\Gamma)$, later chapters.

Notation 4.2.1. For $t > 0$ and $\boldsymbol{u} \in \Gamma$ we write

$$N_t^{\boldsymbol{u}} := \{\boldsymbol{n} \in N^{\boldsymbol{u}} : |\boldsymbol{n}| < t\}, \qquad N_t := \bigcup_{\boldsymbol{v} \in \Gamma} \{\boldsymbol{v}\} \times N_t^{\boldsymbol{v}}.$$

That is, $N_t^{\boldsymbol{u}}$ is a subset of the normal space at $\boldsymbol{u}$ and N_t is a subset of the normal bundle of Γ. For any point $\boldsymbol{z} \in \mathbb{R}^m$ and for any set $\Omega \subseteq \mathbb{R}^m$ we denote

$$B_t(\boldsymbol{z}) := \{\boldsymbol{x} \in \mathbb{R}^m : |\boldsymbol{x} - \boldsymbol{z}| < t\}, \qquad B_t(\Omega) := \{\boldsymbol{x} \in \mathbb{R}^m : \operatorname{dist}(\boldsymbol{x}, \Omega) < t\}.$$

Definition 4.2.2 (See, for example, Lee, 2006, (10.6))**.** Let $\Gamma \subseteq \mathbb{R}^m$ be a C^1 manifold. For each $t > 0$ we define the function e by

$$e : N_t \to B_t(\Gamma), (\boldsymbol{u}, \boldsymbol{n}) \mapsto \boldsymbol{u} + \boldsymbol{n};$$

in other words, e is the exponential map on the normal bundle. We set

$$\operatorname{tub}_t(\Gamma) := e(N_t) = \bigcup_{\boldsymbol{u} \in \Gamma} (\boldsymbol{u} + N_t^{\boldsymbol{u}}).$$

When this union is disjoint, i.e. e is injective on N_t, we say that Γ has a *tubular neighbourhood* of radius t. We denote the largest such radius by

$$\tau(\Gamma) := \max\bigl(\{0\} \cup \{t > 0 : \operatorname{tub}_t(\Gamma) \text{ is a tubular neighbourhood}\}\bigr),$$

and sometimes just write $\operatorname{tub}(\Gamma) := \operatorname{tub}_{\tau(\Gamma)}(\Gamma)$ for the largest tubular neighbourhood.

Remark 4.2.3. One useful property of tubular neighbourhoods that follows immediately from the definition is that for each $\boldsymbol{u} \in \Gamma$ the graph representation $\omega^{\boldsymbol{u}}$ (see Remark 4.1.8) is valid for an open neighbourhood $G^{\boldsymbol{u}}$ of the translated normal ball $\boldsymbol{u} + N_{\tau(\Gamma)}^{\boldsymbol{u}}$, rather than just a neighbourhood of $\boldsymbol{u}$.

Remark 4.2.4. Another useful property of tubular neighbourhoods is that for each point $\boldsymbol{z} \in \operatorname{tub}(\Gamma)$ there is at most one nearest point in Γ (where, as in Remark 4.1.6, a nearest point to $\boldsymbol{z} \in \operatorname{tub}(\Gamma)$ is $\boldsymbol{u} \in \Gamma$ such that $\operatorname{dist}(\boldsymbol{z}, \Gamma) = |\boldsymbol{z} - \boldsymbol{u}|$). To see this, note that if $\boldsymbol{u}, \boldsymbol{v} \in \Gamma$ are nearest points to $\boldsymbol{z}$ then $\boldsymbol{z} - \boldsymbol{u} \in N_{\tau(\Gamma)}^{\boldsymbol{u}}$ and $\boldsymbol{z} - \boldsymbol{v} \in N_{\tau(\Gamma)}^{\boldsymbol{v}}$, so $\boldsymbol{u} = \boldsymbol{v}$ otherwise this would violate the injectivity of e. This idea leads to a significant field of further study called "sets of positive reach"; see §4.4.

Each point $\boldsymbol{z} \in \operatorname{tub}(\Gamma)$ may have no nearest point on Γ at all. To see this, consider a C^∞ curve in $\mathbb{R}^2$ that bends towards itself, such as the Greek letter ρ with a gap added between the curved part and the stem. By our definition of manifolds, this curve does not include its endpoints, so points very close to the end of the curved part have no nearest point, and yet they are in $\operatorname{tub}(\Gamma)$ because they are in the normal space of points in the stem. However, the following remark gives a sufficient condition for nearest points to exist.

Remark 4.2.5. Let Γ be a C^1 manifold. When Γ is also a closed set, each $\boldsymbol{z} \in \mathbb{R}^m$ has <u>at least one</u> nearest point on Γ i.e. there is a point $\boldsymbol{u} \in \Gamma$ such that $|\boldsymbol{z}-\boldsymbol{u}| = \operatorname{dist}(\boldsymbol{z},\Gamma)$. Combined with Remark 4.1.6, which says that $\boldsymbol{z}-\boldsymbol{u} \in N^{\boldsymbol{u}}$, this has some implications on tubular neighbourhoods of Γ:

- For each $t > 0$ (even $t > \tau(\Gamma)$) we have $\operatorname{tub}_t(\Gamma) = B_t(\Gamma)$; in other words, e is surjective. We certainly have $\operatorname{tub}_t(\Gamma) \subseteq B_t(\Gamma)$, so to see their equality note that if $\boldsymbol{z} \in B_t(\Gamma)$ then any nearest point $\boldsymbol{u} \in \Gamma$ satisfies $\boldsymbol{z}-\boldsymbol{u} \in N^{\boldsymbol{u}}$, so $\boldsymbol{z} \in \operatorname{tub}_t(\Gamma)$.

- If $\boldsymbol{z} \in \operatorname{tub}(\Gamma)$ and $\boldsymbol{u} \in \Gamma$ with $\boldsymbol{z}-\boldsymbol{u} \in N^{\boldsymbol{u}}_{\tau(\Gamma)}$ then $\operatorname{dist}(\boldsymbol{z},\Gamma) = |\boldsymbol{z}-\boldsymbol{u}|$ i.e. $\boldsymbol{u}$ is the nearest point to $\boldsymbol{z}$ on Γ. This is the converse statement to Remark 4.1.6 for points in a tubular neighbourhood. To see why this is, note that if not then there is a nearest point $\boldsymbol{v} \in \Gamma$, so $\boldsymbol{z}-\boldsymbol{v} \in N^{\boldsymbol{v}}_{\tau(\Gamma)}$, so $\boldsymbol{u} = \boldsymbol{v}$ otherwise this would violate the injectivity of e. In particular, $(e^{-1}(\boldsymbol{z}))_1$ is the nearest point function and $|(e^{-1}(\boldsymbol{z}))_2|$ is the distance function.

- Finally, the nearest point property will allow us to write the tubular neighbourhood condition as a sphere condition, as shown in the following lemma. This is sometimes taken as the definition of tubular neighbourhoods, as in Gilbarg and Trudinger (1977, Appendix) for example.

Lemma 4.2.6. *Let $\Gamma \subseteq \mathbb{R}^m$ be a closed set and be a C^1 manifold. Let $t > 0$. The following statements are equivalent.*

1. *The set Γ has a tubular neighbourhood of radius t i.e. $t \leqslant \tau(\Gamma)$.*

2. *For each $\boldsymbol{u} \in \Gamma$ and each $\boldsymbol{n} \in N^{\boldsymbol{u}}$ such that $|\boldsymbol{n}| = t$, we have $B_t(\boldsymbol{u}+\boldsymbol{n}) \subseteq \Gamma^{\mathrm{c}}$.*

Proof. <u>2.$\Longleftrightarrow$3.</u> We may rephrase statement 2 as follows.

3. For each $\boldsymbol{u} \in \Gamma$ and each $\boldsymbol{n} \in N^{\boldsymbol{u}}_t$ (i.e. $|\boldsymbol{n}| < t$), we have $B_{|\boldsymbol{n}|}(\boldsymbol{u}+\boldsymbol{n}) \subseteq \Gamma^{\mathrm{c}}$.

These statements are equivalent because, for all $\boldsymbol{u} \in \Gamma$ and $\boldsymbol{n} \in N^{\boldsymbol{u}}$ such that $|\boldsymbol{n}| = 1$, we have

$$B_t(\boldsymbol{u}+t\boldsymbol{n}) = \bigcup_{\lambda \in [0,t)} B_\lambda(\boldsymbol{u}+\lambda\boldsymbol{n}).$$

<u>1.$\Longrightarrow$3.</u> Let $\boldsymbol{u} \in \Gamma$ and $\boldsymbol{n} \in N^{\boldsymbol{u}}_t$, and set $\boldsymbol{z} := \boldsymbol{u}+\boldsymbol{n}$. Then by Remark 4.2.5 (second point), $\operatorname{dist}(\boldsymbol{z},\Gamma) = |\boldsymbol{z}-\boldsymbol{u}| = |\boldsymbol{n}|$; in other words, $B_{|\boldsymbol{n}|}(\boldsymbol{u}+\boldsymbol{n}) \subseteq \Gamma^{\mathrm{c}}$.

2.$\Longrightarrow$1. Assume that statement 1 does not hold: there exist $z \in \mathbb{R}^m$, distinct $\boldsymbol{u}, \boldsymbol{v} \in \Gamma$, $\boldsymbol{n} \in N_t^{\boldsymbol{u}}$ and $\boldsymbol{m} \in N_t^{\boldsymbol{v}}$ such that $\boldsymbol{z} = \boldsymbol{u} + \boldsymbol{n} = \boldsymbol{v} + \boldsymbol{m}$ and without loss of generality $|\boldsymbol{n}| \leqslant |\boldsymbol{m}|$. Then $\boldsymbol{n} \neq \boldsymbol{m}$ so $\boldsymbol{m} \neq \boldsymbol{0}$. Set $\boldsymbol{r} := t\boldsymbol{m}/|\boldsymbol{m}|$, so that $\boldsymbol{r} \in N_{\boldsymbol{v}}$ and $|\boldsymbol{r}| = t$; we will show that $\boldsymbol{u} \in B_t(\boldsymbol{v} + \boldsymbol{r})$, so that $B_t(\boldsymbol{v} + \boldsymbol{r}) \nsubseteq \Gamma^{\mathrm{c}}$, contradicting statement 2. There are two possible cases:

- If $\boldsymbol{n}$ and $\boldsymbol{m}$ are parallel then $\boldsymbol{n} = \lambda \boldsymbol{m}$ where $\lambda \in [-1, 1)$. This implies that

$$|\boldsymbol{u} - (\boldsymbol{v} + \boldsymbol{r})| = |(\boldsymbol{z} - \boldsymbol{n}) - (\boldsymbol{z} - \boldsymbol{m} + \boldsymbol{r})| = |(1-\lambda)\boldsymbol{m} - \boldsymbol{r}| = \Big| t - (1-\lambda)|\boldsymbol{m}| \Big|,$$

  with the final equality holding because $(1-\lambda)\boldsymbol{m}$ and $\boldsymbol{r}$ are parallel. But $1-\lambda > 0$ and $1-\lambda \leqslant 2$, so

$$t - (1-\lambda)|\boldsymbol{m}| < t, \qquad t - (1-\lambda)|\boldsymbol{m}| \geqslant t - 2|\boldsymbol{m}| > 2 - 2t = -t,$$

  so $\Big| t - (1-\lambda)|\boldsymbol{m}| \Big| < t$.

- If $\boldsymbol{n}$ and $\boldsymbol{m}$ are not parallel then

$$|\boldsymbol{u} - (\boldsymbol{v} + \boldsymbol{r})| = |(\boldsymbol{z} - \boldsymbol{n}) - (\boldsymbol{z} - \boldsymbol{m} + \boldsymbol{r})| = \left| \frac{t - |\boldsymbol{m}|}{|\boldsymbol{m}|} \boldsymbol{m} + \boldsymbol{n} \right| < t - |\boldsymbol{m}| + |\boldsymbol{n}| \leqslant t,$$

  where the triangle inequality is strict here because the two vectors are not parallel. $\square$

We now prove the tubular neighbourhood theorem: that a C^2 manifold that is closed and bounded always has a tubular neighbourhood. This is well known fact; see for example Lee (2006, Theorem 10.19), whose proof is essentially followed here.

The proof has three steps. First we use the inverse function theorem to show that around every point in Γ there is a neighbourhood on which the function e (see Definition 4.2.2) is injective. We use the graph representation for this, but neighbourhood might not be the whole of $G^{\boldsymbol{u}}$; for example, $y = \sin x$ has a graph representation on the whole of $\mathbb{R}^2$, but does not have an infinite tubular radius. (It could be argued that the full calculation of the Jacobian in this step is overkill, but it will be needed anyway in the proof of Lemma 4.3.3.) The second step is to shrink each of the neighbourhoods to avoid incompatible maps overlapping; to see why this is necessary, it is helpful to consider points on opposite sides of the neck of an hourglass curve embedded into $\mathbb{R}^2$. The third, and final, step is use a compactness argument with these neighbourhoods to prove the full, global version of the theorem.

Theorem 4.2.7 (Tubular neighbourhood theorem)**.** *Let $\Gamma \subseteq \mathbb{R}^m$ be a closed bounded set and be a C^2 manifold. Then $\tau(\Gamma) > 0$ i.e. there exists a $t > 0$ such that $\operatorname{tub}_t(\Gamma)$ is a tubular neighbourhood.*

Proof. Notation. To avoid a profusion of notation for different sets, for any fixed set A we will write $\widetilde{A}$ for an appropriate subset of A, which will be specified. In the first and second parts of the proof, these sets all depend on which particular point $\boldsymbol{u} \in \Gamma$ we are considering, and will each be a neighbourhood of $\boldsymbol{u}$ or $\boldsymbol{0}$; in the third step, they will each be a neighbourhood of Γ.

The result holds locally. Let $\boldsymbol{u} \in \Gamma$. We will show that e with restricted domain and codomain, denoted by

$$e^{\boldsymbol{u}} : \tilde{N} \to \widetilde{\mathbb{R}^m}, (\boldsymbol{v}, \boldsymbol{m}) \mapsto \boldsymbol{v} + \boldsymbol{m},$$

is bijective. (Here N is the whole normal bundle of Γ i.e. the union of $\{\boldsymbol{v}\} \times N^{\boldsymbol{v}}$ over all $\boldsymbol{v} \in \Gamma$.) We will change coordinates using Remark 4.1.8, which we will denote

$$c^{\boldsymbol{u}} : \widetilde{T^{\boldsymbol{u}} \times N^{\boldsymbol{u}}} \to \tilde{N}, (\boldsymbol{t}, \boldsymbol{n}) \mapsto (\boldsymbol{v}(\boldsymbol{t}), \boldsymbol{m}(\boldsymbol{t}, \boldsymbol{n})),$$

where for each $\boldsymbol{t} \in T^{\boldsymbol{u}}$ and $\boldsymbol{n} \in N^{\boldsymbol{u}}$ we set

$$\boldsymbol{v}(\boldsymbol{t}) := \boldsymbol{u} + \boldsymbol{t} + \omega^{\boldsymbol{u}}(\boldsymbol{t}) \in \Gamma, \qquad \boldsymbol{m}(\boldsymbol{t}, \boldsymbol{n}) := \boldsymbol{n} - \nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}})(\boldsymbol{t}) \in N^{\boldsymbol{v}(\boldsymbol{t})}.$$

By Lemma 4.1.9 the function $c^{\boldsymbol{u}}$ is bijective as a map from $((-\boldsymbol{u} + G^{\boldsymbol{u}}) \cap T^{\boldsymbol{u}}) \times N^{\boldsymbol{u}}$ to the image of this set. The composition $f^{\boldsymbol{u}} := e^{\boldsymbol{u}} \circ c^{\boldsymbol{u}}$ is

$$f^{\boldsymbol{u}} : \widetilde{T^{\boldsymbol{u}} \times N^{\boldsymbol{u}}} \to \widetilde{\mathbb{R}^m}, (\boldsymbol{t}, \boldsymbol{n}) \mapsto \boldsymbol{v}(\boldsymbol{t}) + \boldsymbol{m}(\boldsymbol{t}, \boldsymbol{n}).$$

Rotating so that $T^{\boldsymbol{u}} = \mathbb{R}^k \times \{\mathbf{0}_{m-k}\}$ and $N^{\boldsymbol{u}} = \{\mathbf{0}_k\} \times \mathbb{R}^{m-k}$, we may consider $(\boldsymbol{t}, \boldsymbol{n}) \in \mathbb{R}^m$. Therefore $f^{\boldsymbol{u}}$ is a C^1 map between subsets of $\mathbb{R}^m$, and its Jacobian matrix at $(\boldsymbol{t}, \boldsymbol{n})$ is the block matrix

$$\begin{aligned} \nabla \otimes f^{\boldsymbol{u}}(\boldsymbol{t}, \boldsymbol{n}) &= \begin{pmatrix} \nabla_{\boldsymbol{t}} \otimes (f^{\boldsymbol{u}})_{1,\dots,k} & \nabla_{\boldsymbol{n}} \otimes (f^{\boldsymbol{u}})_{1,\dots,k} \\ \nabla_{\boldsymbol{t}} \otimes (f^{\boldsymbol{u}})_{k+1,\dots,m} & \nabla_{\boldsymbol{n}} \otimes (f^{\boldsymbol{u}})_{k+1,\dots,m} \end{pmatrix} \\ &= \begin{pmatrix} I_k - \nabla_{\boldsymbol{t}} \otimes \nabla_{\boldsymbol{t}}(\boldsymbol{n} \cdot \omega^{\boldsymbol{u}}(\boldsymbol{t})) & -(\nabla_{\boldsymbol{t}} \otimes \omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}} \\ \nabla_{\boldsymbol{t}} \otimes \omega^{\boldsymbol{u}}(\boldsymbol{t}) & I_{m-k} \end{pmatrix}. \end{aligned}$$

Thus at $(\boldsymbol{t}, \boldsymbol{n}) = \mathbf{0}$ the Jacobian determinant is 1, so by the inverse function theorem $f^{\boldsymbol{u}}$ is invertible in a neighbourhood of $\mathbf{0}$. Therefore $e^{\boldsymbol{u}} = f^{\boldsymbol{u}} \circ (c^{\boldsymbol{u}})^{-1}$ is invertible in a neighbourhood of $\boldsymbol{u}$.

Consistency on reduced domains. We may assume that the domain of each $e^{\boldsymbol{u}} : \tilde{N} \to \widetilde{\mathbb{R}^m}$ is of the form

$$\tilde{N} = \{(\boldsymbol{x}, \boldsymbol{m}) \in N : \boldsymbol{x} \in B_{r^{\boldsymbol{u}}}(\boldsymbol{u}), \boldsymbol{m} \in B_{r^{\boldsymbol{u}}}(\mathbf{0})\}$$

for some $r^{\boldsymbol{u}} > 0$ by shrinking it if necessary. We will then consider $e^{\boldsymbol{u}}$ on the reduced domain

$$D^{\boldsymbol{u}} = \{(\boldsymbol{x}, \boldsymbol{m}) \in N : \boldsymbol{x} \in B_{r^{\boldsymbol{u}}/4}(\boldsymbol{u}), \boldsymbol{m} \in B_{r^{\boldsymbol{u}}/4}(\mathbf{0})\}.$$

Let $\boldsymbol{z} \in \mathbb{R}^m$ such that $\boldsymbol{z} \in e^{\boldsymbol{u}}(D^{\boldsymbol{u}})$ and $\boldsymbol{z} \in e^{\boldsymbol{v}}(D^{\boldsymbol{v}})$ for some $\boldsymbol{u}, \boldsymbol{v} \in \Gamma$, and without loss of generality assume $t^{\boldsymbol{v}} > t^{\boldsymbol{u}}$. Then $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{m} = \boldsymbol{y} + \boldsymbol{n}$ where $(\boldsymbol{x}, \boldsymbol{m}) \in D^{\boldsymbol{u}}$ and $(\boldsymbol{y}, \boldsymbol{n}) \in D^{\boldsymbol{v}}$. But

$$|\boldsymbol{x} - \boldsymbol{v}| \leqslant |\boldsymbol{x} - \boldsymbol{z}| + |\boldsymbol{z} - \boldsymbol{y}| + |\boldsymbol{y} - \boldsymbol{v}| = |\boldsymbol{m}| + |\boldsymbol{n}| + |\boldsymbol{y} - \boldsymbol{v}| < \tfrac{1}{4} t^{\boldsymbol{u}} + \tfrac{1}{4} t^{\boldsymbol{v}} + \tfrac{1}{4} t^{\boldsymbol{v}} < t^{\boldsymbol{v}},$$

and we also have $|\boldsymbol{m}| < t^{\boldsymbol{u}} \leqslant t^{\boldsymbol{v}}$, so $(\boldsymbol{x}, \boldsymbol{m})$ is in the (full) domain of $e^{\boldsymbol{v}}$. By the injectivity of $e^{\boldsymbol{v}}$ we therefore have $(\boldsymbol{x}, \boldsymbol{m}) = (\boldsymbol{y}, \boldsymbol{n})$. Since $\boldsymbol{z}$ was arbitrary, we have shown that whenever $\boldsymbol{u}, \boldsymbol{v} \in \Gamma$ are such that $e^{\boldsymbol{u}}(D^{\boldsymbol{u}})$ and $e^{\boldsymbol{v}}(D^{\boldsymbol{v}})$ overlap the functions $e^{\boldsymbol{u}}$ and $e^{\boldsymbol{v}}$ have the same inverse on the intersection of those sets.

The result holds globally. We will show that e is bijective as a function

$$e\colon \widetilde{N} \to \widetilde{\mathbb{R}^m}, (\boldsymbol{u},\boldsymbol{n}) \mapsto \boldsymbol{u}+\boldsymbol{n}, \qquad \widetilde{N} := \bigcup_{\boldsymbol{u}\in\Gamma} D^{\boldsymbol{u}}, \quad \widetilde{\mathbb{R}^m} := \bigcup_{\boldsymbol{u}\in\Gamma} e^{\boldsymbol{u}}(D^{\boldsymbol{u}}).$$

With this domain and codomain, e is surjective because each $e^{\boldsymbol{u}}$ is, and it is injective because of the consistency of different $e^{\boldsymbol{u}}$ that we have just shown. It remains to show that there exists $t>0$ such that $\mathrm{tub}_t(\Gamma)\subseteq\widetilde{\mathbb{R}^m}$.

For each $\boldsymbol{u}\in\Gamma$, let $\delta(\boldsymbol{u}) := \max\{\lambda \geqslant 0 : B_\lambda(\boldsymbol{u}) \subseteq \widetilde{\mathbb{R}^m}\}$. If $\inf_{\boldsymbol{u}\in\Gamma}\delta(\boldsymbol{u}) = 0$ then there exists a sequence $(\boldsymbol{u}_n)_{n=1}^\infty$ such that $\delta(\boldsymbol{u}_n)\to 0$. By the Bolzano–Weierstrass theorem, by passing to a subsequence we have $\boldsymbol{u}_n \to \boldsymbol{v}$ for some $\boldsymbol{v}\in\Gamma$. But $\delta(\boldsymbol{v})>0$ because $\widetilde{\mathbb{R}^m}$ is an open neighbourhood of Γ, so for all sufficiently large n we have $\delta(\boldsymbol{u}_n) > \frac{1}{2}\delta(\boldsymbol{v})$, which contradicts $\delta(\boldsymbol{u}_n)\to 0$. Therefore there must exist some $t>0$ such that $B_t(\Gamma)\subseteq\widetilde{\mathbb{R}^m}$, so by Remark 4.2.5 we have $\mathrm{tub}_t(\Gamma)\subseteq\widetilde{\mathbb{R}^m}$. □

4.3 Curvature

In this section we define the second fundamental form of a manifold and consider some uses of it. This tensor expresses the extrinsic curvature of the manifold i.e. the curvature in a way that depends on how the manifold is embedded in $\mathbb{R}^m$, so that for example a cylinder and a plane embedded in $\mathbb{R}^3$ have different second fundamental forms even though they are locally diffeomorphic. In this section we assume that Γ is a C^2 submanifold of $\mathbb{R}^m$ of dimension k with a tubular radius of $\tau(\Gamma)>0$.

The second fundamental form is usually defined in the abstract setting of Riemannian manifolds (or in the very concrete setting of two-dimensional surfaces in $\mathbb{R}^3$), but a coordinate-based definition can be found, for example, in Milnor (1969, §6), which with the inverse chart $\boldsymbol{t} \mapsto \boldsymbol{u}+\boldsymbol{t}+\omega^{\boldsymbol{u}}(\boldsymbol{t})$ gives the following graph-based definition. This is also the definition used by Gilbarg and Trudinger (1977, Appendix) in codimension 1.

Definition 4.3.1. For each $\boldsymbol{u}\in\Gamma$, define the *second fundamental form* by

$$S^{\boldsymbol{u}}\colon N^{\boldsymbol{u}}\times T^{\boldsymbol{u}}\times T^{\boldsymbol{u}}\to\mathbb{R},\ S^{\boldsymbol{u}}(\boldsymbol{n},\boldsymbol{s},\boldsymbol{t}) := D^2\omega^{\boldsymbol{u}}(\boldsymbol{0},\boldsymbol{s},\boldsymbol{t})\cdot\boldsymbol{n} = (\boldsymbol{s}\cdot\nabla)(\boldsymbol{t}\cdot\nabla)\omega^{\boldsymbol{u}}(\boldsymbol{0})\cdot\boldsymbol{n}.$$

If $\boldsymbol{n}\in N^{\boldsymbol{u}}$ then $S^{\boldsymbol{u}}(\boldsymbol{n})$ is a bilinear form, and where there is no possibility of confusion we also use the notation $S^{\boldsymbol{u}}(\boldsymbol{n})$ to refer to the associated linear map $T^{\boldsymbol{u}}\to T^{\boldsymbol{u}}$, which has the matrix

$$S^{\boldsymbol{u}}(\boldsymbol{n}) = \nabla\otimes\nabla(\boldsymbol{n}\cdot\omega^{\boldsymbol{u}})(\boldsymbol{0}).$$

This is called the *shape operator* or *Weingarten map* associated with $\boldsymbol{n}$. It is real and symmetric and so diagonalizable with an orthogonal set of coordinates; the eigenvalues are called the *principle curvatures associated with $\boldsymbol{n}$*.

The following simple bound relates the size of the shape operator to the tubular radius.

Lemma 4.3.2. Let $\boldsymbol{u} \in \Gamma$, $\boldsymbol{n} \in N^{\boldsymbol{u}}$. The principle curvatures κ_j $(j = 1, \ldots, k)$ associated with $\boldsymbol{n}$ (that is, the eigenvalues of the shape operator) satisfy

$$|\kappa_j| \leqslant \frac{|\boldsymbol{n}|}{\tau(\Gamma)}.$$

It immediately follows that the operator norm of the shape operator satisfies

$$\|S^{\boldsymbol{u}}(\boldsymbol{n})\| \leqslant \frac{|\boldsymbol{n}|}{\tau(\Gamma)}.$$

Proof. By Taylor's theorem, we have as $|\boldsymbol{t}| \to 0$

$$(\boldsymbol{n} \cdot \omega_{\boldsymbol{u}})(\boldsymbol{t}) = \tfrac{1}{2}(\boldsymbol{t} \cdot \nabla)^2 (\boldsymbol{n} \cdot \omega_{\boldsymbol{u}})(\boldsymbol{0}) + o(|\boldsymbol{t}|^2) = \tfrac{1}{2} S_{\boldsymbol{u}}(\boldsymbol{n}, \boldsymbol{t}, \boldsymbol{t}) + o(|\boldsymbol{t}|^2).$$

By choosing $\boldsymbol{t} \in T^{\boldsymbol{u}}$ to be a vector in the direction corresponding to the principle curvature we have $S_{\boldsymbol{u}}(\boldsymbol{n}, \boldsymbol{t}, \boldsymbol{t}) = |\boldsymbol{t}|^2 |\kappa_j|$, so

$$(\boldsymbol{n} \cdot \omega_{\boldsymbol{u}})(\boldsymbol{t}) = \tfrac{1}{2} |\boldsymbol{t}|^2 |\kappa_j| + o(|\boldsymbol{t}|^2).$$

But by Lemma 4.2.6 we have $|(\boldsymbol{n} \cdot \omega_{\boldsymbol{u}})(\boldsymbol{t})| \leqslant |\boldsymbol{n}|\big(\tau(\Gamma) - \sqrt{\tau(\Gamma)^2 - |\boldsymbol{t}|^2}\big) =: \psi(\boldsymbol{t})$ on a sufficiently small neighbourhood of $\boldsymbol{0}$, and ψ satisfies

$$\psi(\boldsymbol{t}) = \frac{1}{2\tau(\Gamma)} |\boldsymbol{n}| |\boldsymbol{t}|^2 + o(|\boldsymbol{t}|^2).$$

Taking the limit as $|\boldsymbol{t}| \to 0$ (while preserving the direction of $\boldsymbol{t}$) gives the stated inequality. $\square$

Our first use of the second fundamental form is to express the Jacobian in the change of variables formula from integrals over a tubular neighbourhood to integrals over the manifold and normal space. As discussed at the start of this chapter, this was originally found by Weyl (1939, §2). The proof here is similar but uses graph coordinates, as done in codimension 1 by Gilbarg and Trudinger (1977, Appendix, proof of Lemma 1).

Lemma 4.3.3. *Let $\Gamma \subseteq \mathbb{R}^m$ be a C^2 manifold of dimension k, let $t > 0$ satisfy $t \leqslant \tau(\Gamma)$, and let $g \in L^1(\mathrm{tub}_t(\Gamma))$. Then we have*

$$\int_{\mathrm{tub}_t(\Gamma)} g(\boldsymbol{z}) \,\mathrm{d}\boldsymbol{z} = \int_\Gamma \int_{N_t^{\boldsymbol{u}}} g(\boldsymbol{u} + \boldsymbol{n}) \det(I_k - S^{\boldsymbol{u}}(\boldsymbol{n})) \mu_{m-k}(\mathrm{d}\boldsymbol{n}) \mu_k(\mathrm{d}\boldsymbol{u}).$$

Proof. Overview. By definition of tubular neighbourhoods, the function $e \colon N_t \to \mathrm{tub}_t(\Gamma)$ is bijective (see Definition 4.2.2), so it remains to find the Jacobian of the change of variables. Let $\boldsymbol{u} \in \Gamma$ and define $e^{\boldsymbol{u}}$, $c^{\boldsymbol{u}}$ and $f^{\boldsymbol{u}}$ as in the proof of Theorem 4.2.7, except that by Remark 4.2.3 we may now assume that $N_t^{\boldsymbol{u}} \subseteq \widetilde{N}$. The Jacobian of $e^{\boldsymbol{u}}$ equals that of e, since they are the same function on an open neighbourhood of $N_t^{\boldsymbol{u}}$. We must therefore find the Jacobians of $f^{\boldsymbol{u}}$ and $c^{\boldsymbol{u}}$, and the Jacobian of $e^{\boldsymbol{u}}$ then follows because $e^{\boldsymbol{u}} = f^{\boldsymbol{u}} \circ (c^{\boldsymbol{u}})^{-1}$. (The key part of the proof is finding the

Jacobian of $f^{\boldsymbol{u}}$. The calculations with $c^{\boldsymbol{u}}$ just verify that we did not lose any information when choosing coordinates.)

Jacobian for $f^{\boldsymbol{u}}$. We have

$$\int_{\widetilde{\mathrm{tub}_t(\Gamma)}} g(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = \int_{\widetilde{T^{\boldsymbol{u}}\times N^{\boldsymbol{u}}}} g(\boldsymbol{v}(\boldsymbol{t})+\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}))\,J_{f^{\boldsymbol{u}}}(\boldsymbol{t},\boldsymbol{n})\,\mathrm{d}(\boldsymbol{t},\boldsymbol{n}),$$

where, as in the proof of Theorem 4.2.7, we have

$$\boldsymbol{v}(\boldsymbol{t}) := \boldsymbol{u}+\boldsymbol{t}+\omega^{\boldsymbol{u}}(\boldsymbol{t})\in\Gamma, \qquad \boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}) := \boldsymbol{n}-\nabla_{\boldsymbol{t}}(\boldsymbol{n}\cdot\omega^{\boldsymbol{u}})(\boldsymbol{t})\in N^{\boldsymbol{v}(\boldsymbol{t})}.$$

We again have the Jacobian matrix

$$\nabla\otimes f^{\boldsymbol{u}}(\boldsymbol{t},\boldsymbol{n}) = \begin{pmatrix} I_k-\nabla_{\boldsymbol{t}}\otimes\nabla_{\boldsymbol{t}}(\boldsymbol{n}\cdot\omega^{\boldsymbol{u}}(\boldsymbol{t})) & -(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}} \\ \nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}) & I_{m-k}\end{pmatrix},$$

so the Jacobian of $f^{\boldsymbol{u}}$ at $(\boldsymbol{0},\boldsymbol{n})$ is

$$J_{f^{\boldsymbol{u}}}(\boldsymbol{0},\boldsymbol{n}) = \det\bigl(\nabla\otimes f^{\boldsymbol{u}}(\boldsymbol{0},\boldsymbol{n})\bigr) = \det(I_k-\nabla\otimes\nabla(\boldsymbol{n}\cdot\omega^{\boldsymbol{u}}(\boldsymbol{0})) = \det(I_k-S^{\boldsymbol{u}}(\boldsymbol{n})).$$

By Lemma 4.3.2 this is strictly greater than zero whenever $|\boldsymbol{n}|<\tau(\Gamma)$.

Jacobian for $c^{\boldsymbol{u}}$. First we use the fact that for any $q\in L^1(\widetilde{\Gamma})$ we have the change of variables formula (see for example Evans and Gariepy, 1992, Theorem 2 in §3.3.3 with Theorem 3 in §3.2.1)

$$\int_{\widetilde{\Gamma}} q(\boldsymbol{v})\mu_k(\mathrm{d}\boldsymbol{v}) = \int_{\widetilde{T^{\boldsymbol{u}}}} q(\boldsymbol{v}(\boldsymbol{t}))J_1(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t},$$

where $J_1(\boldsymbol{t}) = \sqrt{\det(L_1^{\mathrm{T}}L_1)}$ and

$$L_1 := \nabla\otimes\boldsymbol{v}(\boldsymbol{t}) = \begin{pmatrix}\nabla_{\boldsymbol{t}}\otimes(\boldsymbol{v}(\boldsymbol{t}))_{1,\dots,k} \\ \nabla_{\boldsymbol{t}}\otimes(\boldsymbol{v}(\boldsymbol{t}))_{k+1,\dots,m}\end{pmatrix} = \begin{pmatrix} I_k \\ \nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t})\end{pmatrix}.$$

Thus

$$J_1(\boldsymbol{t}) = \sqrt{\det(L_1^{\mathrm{T}}L_1)} = \sqrt{\det\bigl(I_k+(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}}(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))\bigr)},$$

which by Sylvester's determinant identity (see for example Harville, 1997, Corollary 18.1.2) may be written in the alternative form

$$J_1(\boldsymbol{t}) = \sqrt{\det\bigl(I_{m-k}+(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}}\bigr)}.$$

For example, if $k=1$ then $J_1(\boldsymbol{t}) = \sqrt{1+\bigl|\frac{\mathrm{d}}{\mathrm{d}t}\omega^{\boldsymbol{u}}(t)\bigr|^2}$, and if $k=m-1$ (so Γ has codimension 1) then $J_1(\boldsymbol{t}) = \sqrt{1+|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|^2}$. Next we use the fact that for any $p\in L^1(\widetilde{N^{\boldsymbol{v}(\boldsymbol{t})}})$ we have

$$\int_{\widetilde{N^{\boldsymbol{u}}}} p(\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}))J_2(\boldsymbol{t},\boldsymbol{n})\,\mathrm{d}\boldsymbol{n} = \int_{\widetilde{N^{\boldsymbol{v}(\boldsymbol{t})}}} p(\boldsymbol{m})\,\mathrm{d}\boldsymbol{m},$$

where $J_2(\boldsymbol{t},\boldsymbol{n}) = \sqrt{\det(L_2^{\mathrm{T}}L_2)}$ and

$$L_2 := \nabla_{\boldsymbol{n}}\otimes\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}) = \begin{pmatrix}\nabla_{\boldsymbol{n}}\otimes(\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}))_{1,\dots,k} \\ \nabla_{\boldsymbol{n}}\otimes(\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}))_{k+1,\dots,m}\end{pmatrix} = \begin{pmatrix}-(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}} \\ I_{m-k}\end{pmatrix}.$$

Thus

$$J_2(\boldsymbol{t},\boldsymbol{n})=\sqrt{\det(L_2^{\mathrm{T}}L_2)}=\sqrt{\det\big(I_{m-k}+(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}}\big)}=J_1(\boldsymbol{t}).$$

Putting these together, we obtain, for any integrable function r,

$$\begin{aligned}\int_\Gamma\int_{N_t^{\boldsymbol{v}}} & r(\boldsymbol{v},\boldsymbol{m})\mu_{m-k}(\mathrm{d}\boldsymbol{m})\mu_k(\mathrm{d}\boldsymbol{v})\\ &=\int_{\widetilde{T^{\boldsymbol{u}}\times N^{\boldsymbol{u}}}} r(\boldsymbol{v}(\boldsymbol{t}),\boldsymbol{m}(\boldsymbol{t},\boldsymbol{n}))\det\big(I_k+(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))^{\mathrm{T}}(\nabla_{\boldsymbol{t}}\otimes\omega^{\boldsymbol{u}}(\boldsymbol{t}))\big)\mathrm{d}(\boldsymbol{t},\boldsymbol{n}),\end{aligned}$$

and this Jacobian is 1 when $\boldsymbol{t}=\boldsymbol{0}$. □

Our other use of the second fundamental form will be, in codimension 1, to bound the variation in the natural normal field. First we will need some extra notation.

Notation 4.3.4. Let Γ be a C^2 manifold of codimension 1 (i.e. $k=m-1$) that is orientable i.e. there exists some continuous choice of normal field $\boldsymbol{n}\colon\Gamma\to N$, with $|\boldsymbol{n}(\boldsymbol{u})|=1$ at each $\boldsymbol{u}\in\Gamma$. For $\boldsymbol{u}\in\Gamma$ we denote the shape operator associated with $\boldsymbol{n}(\boldsymbol{u})$ simply by

$$S^{\boldsymbol{u}}:=S^{\boldsymbol{u}}(\boldsymbol{n}(\boldsymbol{u}))=\pm(\boldsymbol{s}\cdot\nabla)(\boldsymbol{t}\cdot\nabla)\omega^{\boldsymbol{u}}(\boldsymbol{0}).$$

In particular, for $\lambda\in\mathbb{R}$ we have $S^{\boldsymbol{u}}(\lambda\boldsymbol{n}(\boldsymbol{u}))=\lambda S^{\boldsymbol{u}}$. In the case that $\Gamma=\partial\Omega$ where Ω is a C^2 domain, we choose $\boldsymbol{n}\colon\partial\Omega\to\mathbb{R}^m$ to be the <u>inward</u> normal vector field, and the sign in the above equation is + due to Remark 4.1.10.

Remark 4.3.5. We will commonly use the normal vector field on such a manifold to write any point $\boldsymbol{z}\in\operatorname{tub}(\Gamma)$ as $\boldsymbol{z}=\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})$ where $\boldsymbol{u}=(e^{-1}(\boldsymbol{z}))_1\in\Gamma$ and $|\lambda|<\tau(\Gamma)$. (When Γ is closed, $\boldsymbol{u}$ is the nearest point to $\boldsymbol{z}$ on Γ and $\lambda=\pm\operatorname{dist}(\boldsymbol{z},\partial\Omega)$.) For example, Lemma 4.3.3 then says

$$\int_{\operatorname{tub}_t(\Gamma)}g(\boldsymbol{z})\mathrm{d}\boldsymbol{z}=\int_\Gamma\int_{-t}^{t}g(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))\det(I_k-\lambda S^{\boldsymbol{u}})\mathrm{d}\lambda\,\mu_{m-1}(\mathrm{d}\boldsymbol{u}).$$

Ultimately, we will bound the difference between nearby normals by applying Taylor's theorem on a line directly connecting them. To do this we will first need to extend the normal field from just Γ to a larger set, and then we will need to bound $\nabla\otimes\boldsymbol{n}$. This result is due to Gilbarg and Trudinger (1977, Appendix, Lemma 2), whose proof is followed here.

Notation 4.3.6. Let Γ be an orientable C^2 manifold of dimension $m-1$ with $\tau(\Gamma)>0$, and let $\boldsymbol{n}$ be a continuous unit vector field on it. For each $\boldsymbol{z}\in\operatorname{tub}(\Gamma)$, set

$$\boldsymbol{n}(\boldsymbol{z}):=\boldsymbol{n}\big((e^{-1}(\boldsymbol{z}))_1\big).$$

For each $\boldsymbol{u}\in\Gamma$ this is constant for all $\boldsymbol{z}\in\boldsymbol{u}+N^{\boldsymbol{u}}_{\tau(\partial\Omega)}$, so this extension to the normal vector field satisfies $|\boldsymbol{n}(\boldsymbol{z})|=1$ and $(\boldsymbol{n}(\boldsymbol{z})\cdot\nabla)\boldsymbol{n}(\boldsymbol{z})=\boldsymbol{0}$.

Lemma 4.3.7. *Let Γ be an orientable C^2 manifold of dimension $m-1$ with $\tau(\Gamma)>0$, and let $\boldsymbol{n}$ be a continuous unit vector field on it. Then the extension to $\boldsymbol{n}$ satisfies $\boldsymbol{n}\in C^{r-1}(\operatorname{tub}(\Gamma))$ and for each $\boldsymbol{z}\in\operatorname{tub}(\Gamma)$, writing $\boldsymbol{z}=\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})$, it satisfies*

$$\nabla\otimes\boldsymbol{n}(\boldsymbol{z})=\begin{pmatrix}-S^{\boldsymbol{u}}(I-\lambda S^{\boldsymbol{u}})^{-1} & 0\\ 0 & 0\end{pmatrix}.$$

In particular, we have $\nabla\otimes\boldsymbol{n}(\boldsymbol{u})=-S^{\boldsymbol{u}}\oplus 0$.

Proof. Summary. Let $\boldsymbol{z}\in\operatorname{tub}(\partial\Omega)$ and write $\boldsymbol{z}=\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})$. We define $f^{\boldsymbol{u}}$ as in Theorem 4.2.7. We denote $\xi:=\big((f^{\boldsymbol{u}})^{-1}\big)_{1,\dots,m-1}$ (which is the "nearest point" mapping $\operatorname{tub}(\Gamma)\to\Gamma$ expressed in terms of the corresponding $\boldsymbol{t}\in T^{\boldsymbol{u}}$), and

$$\boldsymbol{\nu}(\boldsymbol{t}):=\frac{\boldsymbol{n}(\boldsymbol{u})-\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})}{\sqrt{1+|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|^2}},$$

so that $\boldsymbol{n}(\boldsymbol{y})=\boldsymbol{\nu}(\xi(\boldsymbol{y}))$ for all $\boldsymbol{y}$ in a neighbourhood of $\boldsymbol{z}$. Thus

$$\nabla\otimes\boldsymbol{n}(\boldsymbol{z})=(\nabla\otimes\boldsymbol{\nu})(\xi(\boldsymbol{z}))\nabla\otimes\xi(\boldsymbol{z}).$$

(The function $\lambda\boldsymbol{\nu}(\boldsymbol{t})$ is similar to $\boldsymbol{m}(\boldsymbol{t},\lambda)$ defined in the proof of Theorem 4.2.7, which is the second component of $c^{\boldsymbol{u}}$; the difference is that $\boldsymbol{\nu}$ is scaled correctly so that it equals the normal field on a neighbourhood of $\boldsymbol{z}$ rather than just at $\boldsymbol{z}$.)

$\nabla\otimes\xi(\boldsymbol{z})$. As in the proof of Theorem 4.2.7, we have

$$\nabla\otimes f^{\boldsymbol{u}}(\boldsymbol{0},\lambda)=\begin{pmatrix}I_{m-1}-\lambda\nabla_{\boldsymbol{t}}\otimes\nabla_{\boldsymbol{t}}\omega^{\boldsymbol{u}}(\boldsymbol{t}) & 0\\ 0 & 1\end{pmatrix}=\begin{pmatrix}I_{m-1}-\lambda S^{\boldsymbol{u}} & 0\\ 0 & 1\end{pmatrix}.$$

This has strictly positive Jacobian when $|\lambda|<\tau(\partial\Omega)$ (as before, this is due to Lemma 4.3.2), so $f^{-1}\in C^{r-1}$ on a neighbourhood of $(\boldsymbol{0},\lambda)$ and

$$(\nabla\otimes(f^{\boldsymbol{u}})^{-1})(\boldsymbol{z})=\begin{pmatrix}(I_{m-1}-\lambda S^{\boldsymbol{u}})^{-1} & 0\\ 0 & 1\end{pmatrix},$$

so $\nabla\otimes\xi(\boldsymbol{z})=\big((I_{m-1}-\lambda S^{\boldsymbol{u}})^{-1},\,0\big)$.

$\nabla\otimes\boldsymbol{\nu}$. Let $a(\boldsymbol{t}):=1/\sqrt{1+|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|^2}$. Then

$$\frac{\partial}{\partial t_i}a(\boldsymbol{t})=-\frac{\frac{\partial}{\partial t_i}|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|^2}{2(1+|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|)^{3/2}}=-\frac{2\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})\cdot\nabla\big(\frac{\partial}{\partial t_i}\omega^{\boldsymbol{u}}(\boldsymbol{t})\big)}{2(1+|\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})|)^{3/2}},$$

so $a(\boldsymbol{0})=1$ and $\nabla a(\boldsymbol{0})=\boldsymbol{0}$. Thus

$$\nabla_{\boldsymbol{t}}\otimes\boldsymbol{\nu}(\boldsymbol{0})=\nabla_{\boldsymbol{t}}\otimes\big(\boldsymbol{n}(\boldsymbol{u})-\nabla\omega^{\boldsymbol{u}}(\boldsymbol{t})\big)\Big|_{\boldsymbol{t}=\boldsymbol{0}}=-\nabla_{\boldsymbol{t}}\otimes\nabla\omega^{\boldsymbol{u}}(\boldsymbol{0})=\begin{pmatrix}-S^{\boldsymbol{u}}\\ 0\end{pmatrix}.$$

Conclusion. We therefore have

$$\nabla\otimes\boldsymbol{n}(\boldsymbol{z})=\begin{pmatrix}-S^{\boldsymbol{u}}\\ 0\end{pmatrix}\big((I_k-\lambda S^{\boldsymbol{u}})^{-1},\,0\big)=\begin{pmatrix}-S^{\boldsymbol{u}}(I_k-\lambda S^{\boldsymbol{u}})^{-1} & 0\\ 0 & 0\end{pmatrix}.$$ □

4.4 Further developments

We have now reviewed some standard theory of tubular neighbourhoods, albeit presented in more detail or with weaker conditions than in most treatments. This is as much standard theory as we will need, but in this section we will briefly note two ways it has been developed beyond this.

The most notable way the theory has been developed is in calculating the volume of tubular neighbourhoods. The change of variables formula Lemma 4.3.3 was originally proved by Weyl (1939, §2) with $g \equiv 1$, which he used to express the volume $\mu_m(\mathrm{tub}_t(\mathit{\Gamma}))$ as a polynomial in t. He then remarked "So far we have hardly done more than what could have been accomplished by any student in a course of calculus." He considered the non-trivial part of his paper to be what came next: a proof that the coefficients of the polynomial could be written in terms of the curvature tensor, which is an intrinsic quantity of the manifold. In other words, it does not depend on the particular embedding in $\mathbb{R}^m$, so that for example a cylinder and a flat plane are (locally) equivalent.

A similar formula was already known for convex bodies, with no regularity requirement. Federer (1959) proved a formula that included both general convex bodies and C^2 manifolds that are closed. The only assumption is that the set have *positive reach*, which is the requirement that there exists a $t > 0$ such that each point in $B_t(\mathit{\Gamma})$ has a unique nearest point on $\mathit{\Gamma}$. This is true for C^1 manifolds that are closed sets with a tubular neighbourhood by Remark 4.2.5, and is true for all convex bodies for all $t > 0$.

Another development of the theory is to study the differentiability of the distance $\mathrm{dist}(\boldsymbol{z}, \mathit{\Gamma})$ considered as a function of $\boldsymbol{z}$. This has been of less widespread interest, but is more similar to the type of theory discussed in this chapter. It was originally considered in low regularity conditions by Federer (1959, Theorem 4.8 (3) and (5)), who showed that for any closed set the distance function is continuously differentiable on the appropriate analogue of a tubular neighbourhood (specifically, the interior of the set U, where U is the set of all points that have a unique nearest point in the set). He also showed an important converse: if the distance function is differentiable at a point then the point is in U, which led to investigation of the regularity of the distance function to give information about the shape of the set (see for example Delfour and Zolésio, 2011, Chapter 6).

For higher regularity manifolds, it is straightforward to see that when $\mathit{\Gamma}$ is a C^r manifold the distance function is C^{r-1} for points in $\mathrm{tub}(\mathit{\Gamma})\backslash\mathit{\Gamma}$: as in the proof of Lemma 4.3.7, we may show that the nearest point function is C^{r-1}, and then the distance function is $|\boldsymbol{z}-\mathrm{near}(\boldsymbol{z}, \mathit{\Gamma})|$. But Gilbarg and Trudinger (1977, Appendix) showed that the distance function is even C^r in codimension 1, and calculated its gradient (which is the unit normal of the nearest point) and Hessian (i.e. $\nabla \otimes \boldsymbol{n}(\boldsymbol{z})$, which is Lemma 4.3.7 in this thesis). The higher codimension version of this result was then proved by Foote (1984). The distance function cannot be differentiable on $\mathit{\Gamma}$ for the same reason that $x \mapsto |x|$ on $\mathbb{R}$ is not differentiable at 0, but in codimension 1 the signed distance function (λ in Remark 4.3.5) is C^r even on $\mathit{\Gamma}$, and in any codimension the square of the distance function is C^r on $\mathit{\Gamma}$; for this reason these are often studied instead of the standard distance function.

4.5 Extensibility

The main result of this thesis will be stated with two sets of assumptions. The first will assume that the domain is C^2, and for this the theory developed in §4.2 and §4.3 is suitable for the geometry of the boundary. The second will assume, roughly speaking, only that the boundary is piecewise C^2 (and also bounded). In that case the theory developed so far will not be sufficient, even for the individual pieces that make up the boundary, so in this section we develop a small modification of the standard theory that will apply in that situation.

The definition of a manifold embedded in Euclidean space that we are using (Definition 4.1.4) and the definition of tubular neighbourhood (Definition 4.2.2) make no requirement that the manifold be a closed set. But the case that the manifold is a closed set is still useful, for at least two reasons:

- When the manifold is closed and also bounded, a compactness argument implies that a tubular neighbourhood exists (see Theorem 4.2.7).
- We will want to manipulate $\operatorname{dist}(\boldsymbol{z},\Gamma)$ as a function of $\boldsymbol{z}$ for all points that are sufficiently close to Γ. For closed Γ, the nearest point property (see Remark 4.2.5) implies that we may use tubular theory to do this, especially because $\operatorname{dist}(\boldsymbol{z},\Gamma) = |(e^{-1}(\boldsymbol{z}))_2|$.

It is helpful to consider two examples of C^∞ manifolds that are not closed sets and compare against these two properties.

Example 4.5.1. Let $\Gamma \subseteq \mathbb{R}^3$ be the square $(0,1)^2 \times \{0\}$.

- The manifold Γ has a has a tubular neighbourhood with $\tau(\Gamma) = \infty$; for each $t > 0$ the set $\operatorname{tub}_t(\Gamma)$ is an open cuboid (and does not include the rounded edges and corners found in $B_t(\Gamma)$). However, this cannot be seen directly from the proof of Theorem 4.2.7, because that requires a compact set with a graph representation about each point.
- Points close to the x-y plane but outside the square (e.g. $\left(2,2,\frac{1}{2}\right)$) have no nearest point in Γ; there is always a nearest point on the closure $\overline{\Gamma}$, but then $\boldsymbol{z}-\boldsymbol{u}$ may not be in $N^{\boldsymbol{u}}$ (assuming we extend the normal field to the edges of $\overline{\Gamma}$ in the obvious way*) so tubular theory does not apply.

However, both of these issues disappear if we consider $\overline{\Gamma}$ as a subset of the x-y plane P. There is then a nearest point $\boldsymbol{u} \in P$ to each $\boldsymbol{z} \in B_t(\Gamma)$ (for any $t > 0$) with $\boldsymbol{z}-\boldsymbol{u} \in N_t^{\boldsymbol{u}}(P)$, and even though the plane is not bounded we will be able to use a compactness argument on $\overline{\Gamma}$ using the graph representation of P about each point in $\overline{\Gamma}$.

*In fact it is possible to define the normal set $N^{\boldsymbol{u}}$ at each point $\boldsymbol{u}$ in an arbitrary closed set Γ (Federer, 1959, Definition 4.4), which is guaranteed to be a cone but not necessarily a subspace, and then for any $\boldsymbol{z} \in \mathbb{R}^m$ and $\boldsymbol{u} \in \Gamma$ such that $\operatorname{dist}(\boldsymbol{z},\Gamma) = |\boldsymbol{z}-\boldsymbol{u}|$ we do have $\boldsymbol{z}-\boldsymbol{u} \in N^{\boldsymbol{u}}$ (Federer, 1959, Theorem 4.8(2)). In the case of the closure of the square, the normal cone of each point along the edges is a closed half plane, and the normal cone of each point on a vertex is a closed quarter space. However, this is too general to be of use to us here.

Example 4.5.2. Let $\mathit{\Gamma} \subseteq \mathbb{R}^3$ be the curved surface of a bounded cone, excluding the vertex, which is a C^∞ manifold. Unlike the square, it is not clear how to extend the normal field to the vertex, and no matter how small we take $t > 0$ the set $\mathrm{tub}_t(\mathit{\Gamma})$ will not be a tubular neighbourhood because normal lines will intersect near the vertex.

A key difference between these two examples is that for the cone there is no C^2 graph on an neighbourhood of the vertex that includes all nearby points on $\mathit{\Gamma}$, whereas there is for each point on the closed square because we may use the graph representation of the plane that it is embedded in. This motivates the following definition, which ensures that we are in a similar situation to the first example.

Definition 4.5.3. A set $\mathit{\Gamma} \subseteq \mathbb{R}^m$ is called a C^r *strongly extensible manifold* of dimension k if it is closure of a bounded non-empty C^r manifold $\mathit{\Gamma}^{(\mathrm{i})}$ of dimension k and is a subset of a C^r manifold $\mathit{\Gamma}^{(\mathrm{o})}$ of dimension k.

(It would perhaps be more sensible to name $\mathit{\Gamma}^{(\mathrm{i})}$ the "strongly extensible manifold", but this name is given to its closure instead for consistency with the next definition.) It turns out that most of the results in this section do not even require that $\mathit{\Gamma}$ be the closure of a manifold $\mathit{\Gamma}^{(\mathrm{i})}$ because sufficient structure is contained in $\mathit{\Gamma}^{(\mathrm{o})}$. For those results, we use the following terminology.

Definition 4.5.4. A set $\mathit{\Gamma} \subseteq \mathbb{R}^m$ is called a C^r *extensible manifold* of dimension k if it is bounded, non-empty, closed, and contained within a C^r manifold $\mathit{\Gamma}^{(\mathrm{o})}$ of dimension k.

We will show that C^r extensible manifolds have the two desired properties stated at the start of this section. For the first, a form of the tubular neighbourhood theorem, we need to make sense of the notion of normal space for extensible manifolds.

Notation 4.5.5. If $\mathit{\Gamma}$ is a C^2 extensible manifold then we define the normal space at each point in it as the normal space of $\mathit{\Gamma}^{(\mathrm{o})}$ at that point i.e.

$$N^{\boldsymbol{u}}(\mathit{\Gamma}) := N^{\boldsymbol{u}}(\mathit{\Gamma}^{(\mathrm{o})}), \qquad N(\mathit{\Gamma}) := \bigcup_{\boldsymbol{u}\in\mathit{\Gamma}} \{\boldsymbol{u}\} \times N^{\boldsymbol{u}}(\mathit{\Gamma}^{(\mathrm{o})}),$$

and similarly for the size-restricted sets $N_t^{\boldsymbol{u}}(\mathit{\Gamma})$ and $N_t(\mathit{\Gamma})$. In particular, we again denote

$$\mathrm{tub}_t(\mathit{\Gamma}) := e(N_t) = \bigcup_{\boldsymbol{u}\in\mathit{\Gamma}} (\boldsymbol{u} + N_t^{\boldsymbol{u}}(\mathit{\Gamma}^{(\mathrm{o})})),$$

which we call a *tubular neighbourhood* when this union is disjoint. In strongly extensible manifolds, for $\boldsymbol{u} \in \mathit{\Gamma}^{(\mathrm{i})}$ we have $N^{\boldsymbol{u}}(\mathit{\Gamma}^{(\mathrm{i})}) = N^{\boldsymbol{u}}(\mathit{\Gamma}^{(\mathrm{o})})$ because the graph representations are locally the same, so there is no ambiguity in just writing $N^{\boldsymbol{u}}$.

In fact, we will not only prove that each extensible manifold has a tubular neighbourhood, but also show that we may extend it by a uniform amount and that extension still has a tubular neighbourhood. To express this fact we will need the following notation.

Notation 4.5.6. Let $\Gamma \subseteq \mathbb{R}^m$ be a C^r extensible manifold. For each $t > 0$ we denote

$$\operatorname{ext}_t(\Gamma) := \Gamma^{(o)} \cap B_t(\Gamma).$$

If Γ is C^r extensible then $\Gamma^{(o)}$ is not uniquely defined, and therefore neither is $\operatorname{ext}_t(\Gamma)$, but we will assume that some choice is used consistently.

Theorem 4.5.7 (Tubular neighbourhood theorem for C^2 extensible manifolds)**.** *If $\Gamma \subseteq \mathbb{R}^m$ is a C^2 extensible manifold then there exists a $\tau > 0$ such that* $\operatorname{tub}_\tau(\operatorname{ext}_\tau(\Gamma))$ *is a tubular neighbourhood.*

Proof. The proof has precisely the same three steps as that of the tubular neighbourhood theorem for compact C^2 manifolds (see Theorem 4.2.7):

1. For each $\boldsymbol{u} \in \Gamma$ we find a neighbourhood about $\boldsymbol{u}$ on which $\Gamma^{(o)}$ is represented as a graph, shrinking it if necessary so that $e^{\boldsymbol{u}}$ is bijective.

2. We then shrink the neighbourhoods further so that each $e^{\boldsymbol{u}}$ is consistent with the other maps for nearby points.

3. Finally, we apply the same compactness argument as before on Γ to find a domain of uniform width on which e is bijective.

As before, this results in a bijective function

$$e : e^{-1}\big(B_t(\Gamma)\big) \to B_t(\Gamma), (\boldsymbol{u}, \boldsymbol{n}) \mapsto \boldsymbol{u} + \boldsymbol{n}.$$

However, now it is not necessarily true that $B_t(\Gamma) = \operatorname{tub}_t(\Gamma)$. Instead, we show that for $\tau := \frac{1}{2}t$ we have $\operatorname{tub}_\tau(\operatorname{ext}_\tau(\Gamma)) \subseteq B_t(\Gamma)$. Let $\boldsymbol{z} \in \operatorname{tub}_\tau(\operatorname{ext}_\tau(\Gamma))$, so that $\boldsymbol{z} = \boldsymbol{u} + \boldsymbol{n}$ where $\boldsymbol{u} \in \operatorname{ext}_\tau(\Gamma)$ and $\boldsymbol{n} \in N_\tau^{\boldsymbol{u}}$. Then

$$\operatorname{dist}(\boldsymbol{z}, \Gamma) \leqslant |\boldsymbol{z} - \boldsymbol{u}| + \operatorname{dist}(\boldsymbol{u}, \Gamma) < 2\tau = t,$$

so $\boldsymbol{z} \in B_t(\Gamma)$. Therefore $\operatorname{tub}_\tau(\operatorname{ext}_\tau(\Gamma))$ is a tubular neighbourhood. □

We are now in a position to prove an analogue of the second property listed at the start of this chapter: points sufficiently close to an extensible manifold have a nearest point on its extension.

Lemma 4.5.8. *Let Γ be a C^0 extensible manifold. Then there exists $s > 0$ such that for each $\boldsymbol{z} \in B_s(\Gamma)$ there exists a point $\boldsymbol{u} \in \operatorname{ext}_{2s}(\Gamma)$ such that*

$$|\boldsymbol{z} - \boldsymbol{u}| = \operatorname{dist}(\boldsymbol{z}, \Gamma^{(o)}) = \operatorname{dist}(\boldsymbol{z}, \operatorname{ext}_{2s}(\Gamma)).$$

Proof. Minimal radius for graph representations. We define, for each $\boldsymbol{u} \in \Gamma$,

$$\delta(\boldsymbol{u}) := \max\{\lambda \geqslant 0 : \Gamma^{(o)} \text{ is graph-type on } B_\lambda(\boldsymbol{u})\}.$$

We may use the same compactness argument as the tubular neighbourhood theorem, noting that if $\boldsymbol{u}_n \to \boldsymbol{v}$ where all $\boldsymbol{u}_n \in \Gamma$ and $\boldsymbol{v} \in \Gamma$ then for all sufficiently large n we have $\delta(\boldsymbol{u}_n) > \frac{1}{2}\delta(\boldsymbol{v})$. It follows that there exists $t > 0$ such that $\delta(\boldsymbol{u}) \geqslant t$ for all $\boldsymbol{u} \in \Gamma$.

Nearest point on $\Gamma^{(o)}$. Choose $s := \frac{1}{4}t$. Let $\boldsymbol{z} \in B_s(\Gamma)$. Because Γ is closed, there exists $\boldsymbol{v} \in \Gamma$ such that $|\boldsymbol{z} - \boldsymbol{v}| = \operatorname{dist}(\boldsymbol{z}, \Gamma) < s$. We have shown that $\Gamma^{(o)}$ is represented as a graph on $\overline{B_{2s}(\boldsymbol{v})}$, so $\Gamma^{(o)} \cap \overline{B_{2s}(\boldsymbol{v})}$ is a non-empty closed set (because it is the graph of a continuous function on a compact domain). Therefore there exists a nearest point $\boldsymbol{u} \in \Gamma^{(o)} \cap \overline{B_{2s}(\boldsymbol{v})}$ to $\boldsymbol{z}$. We now show that $\boldsymbol{u}$ is a nearest point to $\boldsymbol{z}$ on the whole of $\Gamma^{(o)}$. First note that $\boldsymbol{v} \in \Gamma^{(o)} \cap \overline{B_{2s}(\boldsymbol{v})}$ so $|\boldsymbol{z}-\boldsymbol{u}| \leqslant |\boldsymbol{z}-\boldsymbol{v}| < s$. What is more, if $\boldsymbol{u}' \in \Gamma^{(o)}$ satisfies $|\boldsymbol{z} - \boldsymbol{u}'| < |\boldsymbol{z} - \boldsymbol{u}|$ then

$$|\boldsymbol{u}' - \boldsymbol{v}| \leqslant |\boldsymbol{z} - \boldsymbol{v}| + |\boldsymbol{z} - \boldsymbol{u}'| < 2s,$$

so $\boldsymbol{u}' \in \Gamma^{(o)} \cap \overline{B_{2s}(\boldsymbol{v})}$, which would contradict $\boldsymbol{u}$ being a nearest point to $\boldsymbol{z}$ in $\Gamma^{(o)} \cap \overline{B_{2s}(\boldsymbol{v})}$. Thus $\operatorname{dist}(\boldsymbol{z}, \Gamma^{(o)}) = |\boldsymbol{z} - \boldsymbol{u}|$.

Nearest point on $\operatorname{ext}_{2s}(\Gamma)$. We have $\boldsymbol{u} \in \operatorname{ext}_{2s}(\Gamma)$ because

$$\operatorname{dist}(\boldsymbol{u}, \Gamma) \leqslant |\boldsymbol{z} - \boldsymbol{u}| + \operatorname{dist}(\boldsymbol{z}, \Gamma) < 2s.$$

We have already shown that there is no $\boldsymbol{u}' \in \Gamma^{(o)}$ such that $|\boldsymbol{z} - \boldsymbol{u}'| < |\boldsymbol{z} - \boldsymbol{u}|$, so there is certainly no such $\boldsymbol{u}' \in \operatorname{ext}_{2s}(\Gamma)$, so $|\boldsymbol{z} - \boldsymbol{u}| = \operatorname{dist}(\boldsymbol{z}, \operatorname{ext}_{2s}(\Gamma))$. □

Remark 4.5.9 (Analogue of Remark 4.2.5). In §4.2 we noted that if Γ is a closed set then each $\boldsymbol{z} \in \mathbb{R}^m$ has a nearest point on Γ, and that if Γ is also a C^1 manifold then this implies several further properties. Here we note the analogous conclusions for C^1 extensible manifolds, which follow from Lemma 4.5.8.

- The analogue of the first point is the inclusion $B_s(\Gamma) \subseteq \operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$ for sufficiently small $s > 0$ that Lemma 4.5.8 holds (even if $\operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$ is not a tubular neighbourhood). The reason is precisely as before: if $\boldsymbol{z} \in B_s(\Gamma)$ then any nearest point $\boldsymbol{u} \in \operatorname{ext}_{2s}(\Gamma)$ satisfies $\boldsymbol{z} - \boldsymbol{u} \in N^{\boldsymbol{u}}$, so $\boldsymbol{z} \in \operatorname{tub}_t(\Gamma)$.

- We again have a converse of Remark 4.1.6: if $\operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$ is a tubular neighbourhood, and if $\boldsymbol{z} \in B_s(\Gamma)$ and $\boldsymbol{u} \in \operatorname{ext}_{2s}(\Gamma)$ with $\boldsymbol{z} - \boldsymbol{u} \in N_s^{\boldsymbol{u}}$, then $\operatorname{dist}(\boldsymbol{z}, \Gamma) = |\boldsymbol{z} - \boldsymbol{u}|$ i.e. $\boldsymbol{u}$ is the nearest point to $\boldsymbol{z}$ on Γ. Again, the reason is precisely the same as in the closed set case: if $\boldsymbol{u}$ is not a nearest point then the normal from the actual nearest point would intersect that from $\boldsymbol{u}$. This again implies that $(e^{-1}(\boldsymbol{z}))_1$ is the nearest point function and $|(e^{-1}(\boldsymbol{z}))_2|$ is the distance function.

- We have the following analogue of statement 2 in Lemma 4.2.6: For each $\boldsymbol{u} \in \Gamma$ and each $\boldsymbol{n} \in N^{\boldsymbol{u}}$ such that $|\boldsymbol{n}| = s$, we have $B_s(\boldsymbol{u}+\boldsymbol{n}) \subseteq \Gamma^{\mathrm{c}}$. As in the closed set case, it suffices to prove the weaker version (statement 3 in the proof of Lemma 4.2.6), which immediately follows from the previous bullet point.

We now move on to results that need strong extensibility. In both cases, these will be useful when a strongly extensible manifold is a "piece" of a piecewise C^2 boundary of a domain. In order to use tubular theory on that piece as we would a smooth boundary, we will need to show that a normal vector field may be chosen on the piece in agreement with the boundary, which is shown by the next lemma.

Lemma 4.5.10. *If Γ is a C^1 strongly extensible manifold of dimension $m-1$ and $\Gamma \subseteq \partial\Omega$ where Ω is a Lipschitz domain, then for sufficiently small $t > 0$ a continuous unit normal field on* $\mathrm{ext}_t(\Gamma)$ *may be chosen such that it is consistent with the inward normal field on $\Gamma^{(\mathrm{i})}$ (and, in particular,* $\mathrm{ext}_t(\Gamma)$ *is orientable).*

Proof. Summary. We must find a $t > 0$ and a continuous unit normal vector field

$$\boldsymbol{n}\colon \mathrm{ext}_t(\Gamma) \to \mathbb{S}^{m-1},$$

where for each $\boldsymbol{y} \in \Gamma^{(\mathrm{i})}$ we choose $\boldsymbol{n}(\boldsymbol{y})$ to be the unit inward-pointing normal. We will use a similar three-step strategy to the proof of the tubular neighbourhood theorem: first, we find a ball about each point $\boldsymbol{z} \in \Gamma$ on which we can make a continuous choice of $\boldsymbol{n}$; second, we shrink each ball to ensure that they are consistent with other nearby balls; third, we apply a compactness argument to show that this gives a domain of uniform width.

Joint graph representation. We first note that for each $\boldsymbol{u} \in \Gamma$, by choosing a sufficiently small neighbourhood of $\boldsymbol{u}$, both $\partial\Omega$ and $\Gamma^{(\mathrm{o})}$ may be represented as graphs that share the same axis. This is trivial for $\boldsymbol{u} \in \Gamma^{(\mathrm{i})}$, so consider $\boldsymbol{u} \in \Gamma \setminus \Gamma^{(\mathrm{i})}$. Starting with a graph representation of $\partial\Omega$ on a neighbourhood A of $\boldsymbol{u}$, recall that any Lipschitz function has bounded derivative on those points where a derivative exists. This includes those points in $\Gamma^{(\mathrm{i})} \cap A$, and since $\Gamma^{(\mathrm{i})}$ is C^1, the limit of the derivative at $\boldsymbol{u}$ exists and satisfies the same bound, and there is a neighbourhood where it remains bounded. Thus $\Gamma^{(\mathrm{o})}$ may thus be represented as a graph with this axis and neighbourhood. (To see why this requires that Ω is Lipschitz, compare with the graph $y = \sqrt{|x|}$, which is continuous and composed of two C^∞ extensible pieces, but they cannot be represented in a neighbourhood of 0 with the same axis.)

Now within each neighbourhood, there are two choices of continuous unit normal vector field, and we choose the on that is consistent with the inward normal field on $\partial\Omega$. This choice is defined by those points in the neighbourhood of $\boldsymbol{u}$ that are in $\Gamma^{(\mathrm{i})}$, and such points are certainly in the neighbourhood because $\boldsymbol{u} \in \overline{\Gamma^{(\mathrm{i})}}$, so there are points in $\Gamma^{(\mathrm{i})}$ arbitrarily close to $\boldsymbol{u}$. Another way to state this rule is that if the codomain axis of the graph representation is $\boldsymbol{a}$ then we choose each unit normal such that its inner product with $\boldsymbol{a}$ is positive (see Remark 4.1.10).

Consistency of normal choice. We may assume that the neighbourhood about each $\boldsymbol{u} \in \Gamma$ is a ball, and we denote its radius by $r^{\boldsymbol{u}}$. For each $\boldsymbol{y} \in \Gamma^{(\mathrm{o})}$ that is in at least one of these balls, the discussion above gives a continuous choice of normal field in a neighbourhood of $\boldsymbol{y}$ so long as the same ball is used for all the choices in that neighbourhood. We now show that if we instead consider balls with radii $\frac{1}{2}r^{\boldsymbol{u}}$, then the normal choice for each $\boldsymbol{y}$ in at least one of these balls is independent of the ball used. If $\boldsymbol{y} \in B_{r^{\boldsymbol{u}}/2}(\boldsymbol{u})$ and $\boldsymbol{y} \in B_{r^{\boldsymbol{v}}/2}(\boldsymbol{v})$ for some $\boldsymbol{v} \neq \boldsymbol{u}$ then

$$|\boldsymbol{u}-\boldsymbol{v}| \leq |\boldsymbol{u}-\boldsymbol{y}|+|\boldsymbol{y}-\boldsymbol{v}| < \tfrac{1}{2}(r^{\boldsymbol{u}}+r^{\boldsymbol{v}})$$

so either $\boldsymbol{v} \in B_{r^{\boldsymbol{u}}}(\boldsymbol{u})$ or $\boldsymbol{u} \in B_{r^{\boldsymbol{v}}}(\boldsymbol{v})$; without loss of generality, assume the former, and then the continuous choice of normal field on $B_{r^{\boldsymbol{u}}}(\boldsymbol{u})$, including the points in $\Gamma^{(\mathrm{i})}$ arbitrarily choice to $\boldsymbol{v}$, show that the two graph representations give the same choice of normal at $\boldsymbol{y}$.

Uniform width of set. We have now made a continuous choice of normal field on the set

$$A = \Gamma^{(\mathrm{o})} \cap \bigcup_{\boldsymbol{u}\in\Gamma} B_{r^{\boldsymbol{u}}/2}(\boldsymbol{u}).$$

For each $\boldsymbol{v} \in \Gamma$, let $\delta(\boldsymbol{u}) := \max\{\lambda \geqslant 0 : B_{r^{\boldsymbol{u}}/2}(\boldsymbol{u}) \subseteq A\}$. By exactly the same compactness argument as before, there exists $t > 0$ such that $\delta(\boldsymbol{u}) \geqslant t$ for all $\boldsymbol{u} \in \Gamma$. Thus $\operatorname{ext}_t(\Gamma) \subseteq A$. □

So far in this section, we have established that if the boundary of a domain Ω contains an extensible manifold Γ then Γ may be uniformly extended to a slightly larger C^2 manifold $\operatorname{ext}_{2s}(\Gamma)$. We will need slightly more than this: roughly speaking, the domain Ω may be extended in a way that appears to be a C^2 domain Ω_Γ near to Γ. This is made precise by the following lemma. It may be that Ω_Γ does not match Ω on the whole of the tubular neighbourhood about Γ (if $\partial\Omega$ includes an acute angle), so there is a condition that requires the point of interest to be far away from other parts of the boundary. When applying this lemma, we will make use of the cusp-free property proved in §6.3 to show that this only happens near to the "corners" $\partial^2\Omega$.

Lemma 4.5.11. *Let $\Omega \subseteq \mathbb{R}^m$ be a bounded Lipschitz domain satisfying $\partial\Omega = \Gamma \cup V$ where Γ is strongly C^2-extensible and V is a closed set. Let $s > 0$ be sufficiently small that the conclusion of Theorem 4.5.7 holds (with $\tau = 2s$), the conclusion of Lemma 4.5.8 holds, and the conclusion of Lemma 4.5.10 holds (with $t = 2s$). Using the normal field defined on $\operatorname{ext}_{2s}(\Gamma)$ in Lemma 4.5.10, define*

$$\Omega_\Gamma := \big\{\boldsymbol{u} + \lambda \boldsymbol{n}(\boldsymbol{u}) : \boldsymbol{u} \in \operatorname{ext}_{2s}(\Gamma), \lambda \in [0,s)\big\}.$$

In particular, $\Omega_\Gamma \subseteq \operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$ (indeed it is the "half tube" of radius s about $\operatorname{ext}_{2s}(\Gamma)$). Set $\Lambda := \operatorname{tub}_{s/2}(\Gamma^{(\mathrm{i})})$. Then for each $\boldsymbol{z} \in \Lambda$ we have

$$\operatorname{dist}(\boldsymbol{z}, \partial(\Omega_\Gamma)) = \operatorname{dist}(\boldsymbol{z}, \Gamma).$$

For each $\boldsymbol{z} \in \Lambda$ such that $\operatorname{dist}(\boldsymbol{z},\Gamma) < \operatorname{dist}(\boldsymbol{z}, V)$, setting $\ell^{\boldsymbol{z}} := \min\big\{\frac{1}{2}s, \operatorname{dist}(\boldsymbol{z}, V)\big\}$, we have

$$\Omega_\Gamma \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z}) = \Omega \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z}).$$

Proof. Preliminary fact. We first show that for every $\boldsymbol{z} \in \mathrm{tub}_s(\mathrm{ext}_{2s}(\Gamma))$ (including every $\boldsymbol{z} \in B_s(\Gamma)$), we have

$$\boldsymbol{z} \in \partial(\Omega_\Gamma) \Longleftrightarrow \boldsymbol{z} \in \mathrm{ext}_{2s}(\Gamma).$$

Let $\boldsymbol{z} \in \mathrm{tub}_s(\mathrm{ext}_{2s}(\Gamma))$. We may write $\boldsymbol{z} = \boldsymbol{u} + \lambda \boldsymbol{n}(\boldsymbol{u})$ where $\boldsymbol{u} \in \mathrm{ext}_{2s}(\Gamma)$ and $|\lambda| < s$. If $\lambda = 0$ then $\boldsymbol{z} \in \partial(\Omega_\Gamma)$ (because there are arbitrarily close points in Ω_Γ and $\Omega_\Gamma^{\mathrm{c}}$) and $\boldsymbol{z} \in \mathrm{ext}_{2s}(\Gamma)$. If $\lambda > 0$ then $\boldsymbol{z} \notin \partial(\Omega_\Gamma)$ (because $\boldsymbol{z}$ and all sufficiently nearby points are in Ω_Γ) and $\boldsymbol{z} \notin \mathrm{ext}_{2s}(\Gamma)$. Similarly, if $\lambda < 0$ then $\boldsymbol{z} \notin \partial(\Omega_\Gamma)$ and $\boldsymbol{z} \notin \mathrm{ext}_{2s}(\Gamma)$. This proves the claim.

$\mathrm{dist}(\boldsymbol{z}, \partial(\Omega_\Gamma)) = \mathrm{dist}(\boldsymbol{z}, \Gamma)$. We now prove the first equality in the lemma statement. Let $\boldsymbol{z} \in \Lambda$. Let $\boldsymbol{u} \in \Gamma$ be the nearest point to $\boldsymbol{z}$ on $\mathrm{ext}_{2s}(\Gamma)$ and set $d := \mathrm{dist}(\boldsymbol{z}, \Gamma) = |\boldsymbol{z} - \boldsymbol{u}|$. We certainly have $\mathrm{dist}(\boldsymbol{z}, \partial(\Omega_\Gamma)) \leqslant d$ because $\boldsymbol{u} \in \partial(\Omega_\Gamma)$ by the identity just proved. But we also have, using the second point in Remark 4.5.9,

$$B_d(\boldsymbol{z}) \subseteq B_{s/2}(\boldsymbol{z}) \subseteq B_s(\Gamma) \subseteq \mathrm{tub}_s(\mathrm{ext}_{2s}(\Gamma)),$$

so if there exists $\boldsymbol{y} \in B_d(\boldsymbol{z}) \cap \partial(\Omega_\Gamma)$ then $\boldsymbol{y} \in B_d(\boldsymbol{z}) \cap \mathrm{ext}_{2s}(\Gamma)$, which would contradict $\boldsymbol{u}$ being the nearest point.

$\Omega_\Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$ summary. We will first show that $\partial(\Omega_\Gamma) \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \partial\Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$, which we do by showing that each of these two sets equals $\Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$. We will then use this fact to prove that $\Omega_\Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$.

$\partial\Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$. We certainly have

$$\Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) \subseteq \partial\Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}).$$

To see the reverse inclusion note that for each $\boldsymbol{x} \in \partial\Omega \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$, either $\boldsymbol{x} \in \Gamma$ or $\boldsymbol{x} \in V$, but we also have $\mathrm{dist}(\boldsymbol{z}, V) > 0$ so $\boldsymbol{x} \notin V$, which proves that $\boldsymbol{x} \in \Gamma$.

$\partial(\Omega_\Gamma) \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \Gamma \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$. We have $B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) \subseteq B_s(\Gamma)$, so by the preliminary fact we have

$$\partial(\Omega_\Gamma) \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}) = \mathrm{ext}_{2s}(\Gamma) \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z}).$$

Let $\boldsymbol{y} \in \mathrm{ext}_{2s}(\Gamma) \cap B_{\ell_{\boldsymbol{z}}}(\boldsymbol{z})$; it remains to show that $\boldsymbol{y} \in \Gamma$. Assume $\boldsymbol{y} \notin \Gamma$. Define the line segment

$$\gamma(\boldsymbol{z}, \boldsymbol{y}) := \{\lambda \boldsymbol{z} + (1 - \lambda)\boldsymbol{y} \in \mathbb{R}^m : \lambda \in [0, 1]\}.$$

This satisfies $\gamma(\boldsymbol{z}, \boldsymbol{y}) \subseteq B_s(\Gamma)$, so each point on $\gamma(\boldsymbol{z}, \boldsymbol{y})$ has a unique nearest point on $\mathrm{ext}_{2s}(U)$. Let $\boldsymbol{x} \in \gamma(\boldsymbol{z}, \boldsymbol{y})$ and its unique nearest point $\boldsymbol{w}$ on $\mathrm{ext}_{2s}(\Gamma)$ be the points corresponding to the maximum λ such that $\boldsymbol{w} \in \Gamma$. It then follows that $\boldsymbol{w} \in V$. (To see this, use a graph representation for $\partial\Omega$ in a neighbourhood of $\boldsymbol{w}$. By assumption we do not have $\boldsymbol{y} = \boldsymbol{w}$, so $\lambda \neq 1$. Using the graph representation and continuing in the direction of larger λ we may therefore find points arbitrarily close to $\boldsymbol{w}$ in $\partial\Omega \setminus \Gamma \subseteq W$.) We have

$$|\boldsymbol{z} - \boldsymbol{y}| = |\boldsymbol{z} - \boldsymbol{x}| + |\boldsymbol{x} - \boldsymbol{y}|.$$

But $|\boldsymbol{x}-\boldsymbol{y}| > |\boldsymbol{x}-\boldsymbol{w}|$ because $\boldsymbol{w}$ is the unique nearest point to $\boldsymbol{x}$, so

$$|\boldsymbol{z}-\boldsymbol{y}| > |\boldsymbol{z}-\boldsymbol{x}|+|\boldsymbol{x}-\boldsymbol{w}| \geqslant |\boldsymbol{z}-\boldsymbol{w}| \geqslant \operatorname{dist}(\boldsymbol{z}, V),$$

which contradicts $\boldsymbol{y} \in B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z})$. Therefore if $\boldsymbol{y} \in \operatorname{ext}_{2s}(\Gamma) \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z})$ then $\boldsymbol{y} \in \Gamma$.

$\underline{\Omega_\Gamma \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z}) = \Omega \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z})\text{ conclusion.}}$ Let $\boldsymbol{z} \in \Lambda$ and $\boldsymbol{y} \in B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z})$, and let $\boldsymbol{u} \in \Gamma^{(\mathrm{i})}$ be the nearest point of $\boldsymbol{z}$ to $\Gamma^{(\mathrm{o})}$. We will show that $\boldsymbol{y} \in \Omega_\Gamma$ if and only if $\boldsymbol{y} \in \Omega$ by finding a path from $\boldsymbol{u}$ to $\boldsymbol{y}$, consisting of two line segments, and show that each point on the path that is in either $\partial(\Omega_\Gamma)$ or $\partial\Omega$ is contained in a neighbourhood in which Ω_Γ and Ω agree. Specifically, we will make use of the fact that there is a neighbourhood A of $\Gamma \setminus V$ such that $\Omega_\Gamma \cap A = \Omega \cap A$ (because there is a neighbourhood of each point in $\Gamma \setminus V$ in which $\Gamma^{(\mathrm{o})}$ and $\partial\Omega$ share a graph representation, so by Lemma 4.5.10 they share an epigraph representation in that neighbourhood).

First consider the line segment from $\boldsymbol{u}$ to $\boldsymbol{z}$. In this line segment, only $\boldsymbol{u} \in \partial(\Omega_\Gamma)$ (by the preliminary fact), which is in A. It is also true that $\boldsymbol{u}$ is the only point in $\partial\Omega$ that is in this line segment: Let $\boldsymbol{x}$ be in this line segment and in $\partial\Omega$; if $\boldsymbol{x} \in \Gamma$ then $\boldsymbol{x} \in \Gamma^{(\mathrm{i})}$ so $\boldsymbol{x} = \boldsymbol{u}$ because Λ is a tubular neighbourhood, otherwise $\boldsymbol{x} \in V$, which is not possible because of the assumption that $\operatorname{dist}(\boldsymbol{z}, \Gamma) < \operatorname{dist}(\boldsymbol{z}, V)$. Now consider the line segment from $\boldsymbol{z}$ to $\boldsymbol{y}$. We proved above that each point $\boldsymbol{x}$ on this line is in $\partial(\Omega_\Gamma)$ or $\partial\Omega$ if and only if it is in Γ. When we do have $\boldsymbol{x} \in \Gamma$, we may not have $\boldsymbol{x} \in V$ (because $\ell^{\boldsymbol{z}} \leqslant \operatorname{dist}(\boldsymbol{z}, V)$) so $\boldsymbol{x} \in \Gamma \setminus V$, so $\boldsymbol{z} \in A$. □

4.6 Some basic consequences

So far in this chapter we have covered some of the standard (albeit not always well documented) theory of tubular neighbourhoods (§4.2 and §4.3) and a fairly general minor extension of the standard theory (§4.5). In this section we use this to establish some more specific results that we need for proving the main result of this thesis. They are all straightforward consequences of the theory established already, and fall into three categories:

- Bounds on the Jacobian of tubular change of variables and $\nabla \otimes \boldsymbol{n}$, using the expressions for them established in §4.3 and the bound on the shape operator in Lemma 4.3.2.
- Bounds on two types of function that show that they are concentrated near to a manifold.
- Bounds on integrals of functions that are concentrated near to a manifold.

We begin with two bounds on the Jacobian of the change of variables formula established in Lemma 4.3.3. This is approximately equal to 1 on Γ, so it is bounded (below as well as above) on $\operatorname{tub}_{\tau(\Gamma)/2}(\Gamma)$, and when close to Γ it is close to 1.

Lemma 4.6.1. *Let Γ be a C^2 manifold and $\boldsymbol{u} \in \Gamma$. For $\boldsymbol{n} \in N^{\boldsymbol{u}}$ such that $|\boldsymbol{n}| \leqslant \frac{1}{2}\tau(\Gamma)$ we have*

$$\left(\tfrac{1}{2}\right)^k \leqslant \det(I_k - S^{\boldsymbol{u}}(\boldsymbol{n})) \leqslant \left(\tfrac{3}{2}\right)^k.$$

Proof. Choose an orthogonal set of coordinates that diagonalises $S^{\boldsymbol{u}}(\boldsymbol{n})$, so that

$$S^{\boldsymbol{u}}(\boldsymbol{n}) = \operatorname{diag}\{\kappa_1, \dots, \kappa_k\}.$$

Thus

$$\det(I_k - S^{\boldsymbol{u}}(\boldsymbol{n})) = (1-\kappa_1)\cdots(1-\kappa_k),$$

where by Lemma 4.3.2 each κ_j satisfies $|\kappa_j| \leqslant \frac{1}{2}$ so $\frac{1}{2} \leqslant (1-\kappa_j) \leqslant \frac{3}{2}$. □

Lemma 4.6.2. *Let Γ be a C^2 manifold and $\boldsymbol{u} \in \Gamma$. For $\boldsymbol{n} \in N^{\boldsymbol{u}}$ such that $|\boldsymbol{n}| < \tau(\Gamma)$ we have*

$$\left|\det(I_k - S^{\boldsymbol{u}}(\boldsymbol{n})) - 1\right| \leqslant (2^k - 1)\frac{|\boldsymbol{n}|}{\tau(\Gamma)}.$$

Proof. As in the proof of Lemma 4.6.1, choose coordinates so that $S^{\boldsymbol{u}}(\boldsymbol{n})$ is diagonalised. Denote $P := \{0,1\}^k$. Then

$$\begin{aligned}
\det(I - S^{\boldsymbol{u}}(\boldsymbol{n})) - 1 &= \left(\prod_{j=1}^{k}(1-\kappa_k)\right) - 1 \\
&= \left(\sum_{\boldsymbol{p}\in P}(-1)^{|\boldsymbol{p}|}\kappa_1^{p_1}\cdots\kappa_k^{p_k}\right) - 1 \\
&= \sum_{\boldsymbol{p}\in P\setminus\{\boldsymbol{0}\}}(-1)^{|\boldsymbol{p}|}\kappa_1^{p_1}\cdots\kappa_k^{p_k}.
\end{aligned}$$

Every term in this sum contains at least one κ_j raised to the power 1, which by Lemma 4.3.2 satisfies

$$|\kappa_j| \leqslant \frac{|\boldsymbol{n}|}{\tau(\Gamma)}.$$

The remaining $|\kappa_j^{p_j}|$ in the product either equal 1 if $p_j = 0$ or are bounded by 1 if $p_j = 1$ (again by Lemma 4.3.2). There are $2^k - 1$ terms, so the stated inequality follows. □

In a similar way we bound the expression for $\nabla \otimes \boldsymbol{n}$ found in Lemma 4.3.7.

Lemma 4.6.3. *Let Γ be an orientable C^2 manifold of dimension $m-1$ with $\tau(\Gamma) > 0$, and let $\boldsymbol{n}$ be a continuous unit vector field on it. Then for all $\boldsymbol{z} \in \operatorname{tub}_{\tau(\Gamma)/2}(\Gamma)$ we have the operator norm bound*

$$\|\nabla \otimes \boldsymbol{n}(\boldsymbol{z})\| \leqslant \frac{2}{\tau(\partial\Omega)}.$$

Proof. Write $\boldsymbol{z} = \boldsymbol{u} + \lambda\boldsymbol{n}(\boldsymbol{u})$ where $\boldsymbol{u} \in \Gamma$. In coordinates that diagonalise $S^{\boldsymbol{u}}$, by Lemma 4.3.7

$$\nabla \otimes \boldsymbol{n}(\boldsymbol{z}) = \operatorname{diag}\left\{\frac{-\kappa_1}{1-\lambda\kappa_1}, \dots, \frac{-\kappa_{m-1}}{1-\lambda\kappa_{m-1}}, 0\right\}.$$

But $|\lambda| < \frac{1}{2}\tau(\Gamma)$, so by Lemma 4.3.2 we have $|\lambda| < 1/2|\kappa_j|$ for each j. Thus

$$\|\nabla \otimes \boldsymbol{n}(\boldsymbol{z})\| = \max_{j=1,\dots,m-1}\left|\frac{-\kappa_j}{1-\lambda\kappa_j}\right| \leqslant \max_{j=1,\dots,m-1} 2|\kappa_j| \leqslant \frac{2}{\tau(\partial\Omega)}.$$ □

We now turn our attention to two functions that are concentrated near to a manifold. The first is the product of a function that decays away from a domain Ω with a function that decays away from its complement Ω^{c}; the result is a function that decays away from $\partial\Omega$. In fact its proof does not require any tubular theory, but it will be applied in a tubular context (particularly to express $\operatorname{dist}(\boldsymbol{z},\partial\Omega)$ as $|(e^{-1}(\boldsymbol{z}))_2|$).

Notation 4.6.4. We will need to refer to functions that have quick decay properties like Schwartz functions but are not necessarily smooth; that is,

$$Q(\Omega) := \left\{ f \in L^\infty(\Omega) \,\middle|\, \forall n \in \mathbb{N}_0 : \exists c_n \in \mathbb{R}_+ \text{ s.t. } \forall \boldsymbol{x} \in \Omega : |f(\boldsymbol{x})| \leqslant c_n / \langle \boldsymbol{x} \rangle^n \right\}.$$

Lemma 4.6.5. *Let $\Omega \subseteq \mathbb{R}^m$ be any set and let $V \in Q(\mathbb{R}^m)$. Then there exists a decreasing function $\psi_V \in Q(\mathbb{R}_+)$ depending on V but not Ω, such that for each $\boldsymbol{z} \in \mathbb{R}^m$ we have*

$$|V * \chi_\Omega(\boldsymbol{z}) V * \chi_{\Omega^{\mathrm{c}}}(\boldsymbol{z})| \leqslant \psi_V(\operatorname{dist}(\boldsymbol{z},\partial\Omega)).$$

Furthermore, if $\operatorname{supp} V \subseteq B_t(\mathbf{0})$ *for some* $t > 0$ *then* $\operatorname{supp}\psi_V \subseteq [0,t]$. *Finally, if $U \in Q(\mathbb{R}^m)$ such that $|U(\boldsymbol{z})| \geqslant |V(\boldsymbol{z})|$ for each $\boldsymbol{z} \in \mathbb{R}^m$ then $\psi_U(\lambda) \geqslant \psi_V(\lambda)$ for each $\lambda \in \mathbb{R}_+$.*

Proof. For $\boldsymbol{z} \in \Omega^{\mathrm{c}}$ we have $B_{\operatorname{dist}(\boldsymbol{z},\Omega)}(\boldsymbol{z}) \subseteq \Omega^{\mathrm{c}}$, so

$$\Omega \subseteq B_{\operatorname{dist}(\boldsymbol{z},\Omega)}(\boldsymbol{z})^{\mathrm{c}} = B_{\operatorname{dist}(\boldsymbol{z},\partial\Omega)}(\boldsymbol{z})^{\mathrm{c}}.$$

Thus, denoting $\Theta := B_{\operatorname{dist}(\boldsymbol{z},\partial\Omega)}(\mathbf{0})^{\mathrm{c}}$,

$$\begin{aligned}
|V * \chi_\Omega(\boldsymbol{z})| &\leqslant \int_{\mathbb{R}^m} \chi_\Omega(\boldsymbol{z}-\boldsymbol{z}')|V(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}' \\
&\leqslant \int_{\mathbb{R}^m} \chi_{(\boldsymbol{z}+\Theta)}(\boldsymbol{z}-\boldsymbol{z}')|V(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}' \\
&= \int_{\mathbb{R}^m} \chi_\Theta(-\boldsymbol{z}')|V(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}' \\
&= V_{\mathrm{rad}}(\operatorname{dist}(\boldsymbol{z},\partial\Omega)), \quad \text{where } V_{\mathrm{rad}}(\lambda) := \int_{|\boldsymbol{z}'|\geqslant\lambda} |V(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.
\end{aligned}$$

We also have $|V * \chi_{\Omega^{\mathrm{c}}}(\boldsymbol{z})| \leqslant \int |V(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} = V_{\mathrm{rad}}(0)$, and similarly when $\boldsymbol{z} \in \Omega$ we have $|V * \chi_{\Omega^{\mathrm{c}}}(\boldsymbol{z})| \leqslant V_{\mathrm{rad}}(\operatorname{dist}(\boldsymbol{z},\partial\Omega))$ and $|V * \chi_\Omega(\boldsymbol{z})| \leqslant V_{\mathrm{rad}}(0)$. Setting $\psi(t) := V_{\mathrm{rad}}(0)V_{\mathrm{rad}}(t)$ gives the stated bound and it satisfies the further stated properties. □

The function in the next lemma is also concentrated near to a manifold Γ. The function could be considered as something like $V *$"δ_Γ", where δ_Γ is a generalisation of the Dirac delta function whose integral over $\mathbb{R}^m$ gives the surface integral over Γ. The trick used is to thicken Γ into a fixed-sized tube $\operatorname{tub}_{1/2}(\Gamma)$, and note that the distance from that is a fixed amount less than the distance from Γ.

Lemma 4.6.6. *Let $V \in Q(\mathbb{R}^m)$. Let Γ be C^2 manifold with $\tau(\Gamma) \geqslant 1$. Then there exists a decreasing function $\psi_V \in Q(\mathbb{R}_+)$ depending on V but not Γ, such that for each $\boldsymbol{z} \in \mathbb{R}^m$ we have*

$$\int_\Gamma |V(\boldsymbol{z}-\boldsymbol{u})|\,\mu_k(\mathrm{d}\boldsymbol{u}) \leqslant \psi_V(\mathrm{dist}(\boldsymbol{z},\Gamma)).$$

Furthermore, if $\operatorname{supp} V \subseteq B_t(\mathbf{0})$ *for some* $t>0$ *then* $\operatorname{supp}\psi_V \subseteq [0,t+1]$. *Finally, if $U \in Q(\mathbb{R}^m)$ such that $|U(\boldsymbol{z})| \geqslant |V(\boldsymbol{z})|$ for each $\boldsymbol{z}\in\mathbb{R}^m$ then $\psi_U(\lambda) \geqslant \psi_V(\lambda)$ for each $\lambda \in \mathbb{R}_+$.*

Proof. For each $\boldsymbol{y} \in \mathbb{R}^m$ set

$$\widetilde{V}(\boldsymbol{y}) := \sup_{\boldsymbol{x}\in B_{1/2}(\boldsymbol{y})} |V(\boldsymbol{x})|,$$

so that $\widetilde{V} \in Q(\mathbb{R}^m)$ and if $\operatorname{supp} V \subseteq B_t(\mathbf{0})$ then $\operatorname{supp}\widetilde{V} \subseteq B_{t+1/2}(\mathbf{0})$. Then by Lemma 4.3.3 and Lemma 4.6.1 we have

$$\begin{aligned}\int_\Gamma |V(\boldsymbol{z}-\boldsymbol{u})|\,\mu_k(\mathrm{d}\boldsymbol{u}) &\leqslant \frac{2^k}{C_{m-k}}\int_{\mathrm{tub}_{1/2}(\Gamma)} \widetilde{V}(\boldsymbol{z}-\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'\\ &\leqslant \frac{2^k}{C_{m-k}}\int_{B_{1/2}(\Gamma)} \widetilde{V}(\boldsymbol{z}-\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'\\ &= \frac{2^k}{C_{m-k}}\int_{\mathbb{R}^m} \chi_{B_{1/2}(\Gamma)}(\boldsymbol{z}-\boldsymbol{z}')\widetilde{V}(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',\end{aligned}$$

where C_{m-k} is the volume of the $(m-k)$-dimensional ball of radius $\frac{1}{2}$. For $\boldsymbol{z} \notin B_{1/2}(\Gamma)$, treating $B_{1/2}(\Gamma)$ as we did Ω^{c} in Lemma 4.6.5, we have

$$\int_{\mathbb{R}^m} \chi_{B_{1/2}(\Gamma)}(\boldsymbol{z}-\boldsymbol{z}')\widetilde{V}(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' \leqslant \widetilde{V}_{\mathrm{rad}}\big(\mathrm{dist}(\boldsymbol{z},B_{1/2}(\Gamma))\big) = \widetilde{V}_{\mathrm{rad}}\big(\mathrm{dist}(\boldsymbol{z},\Gamma)-\tfrac{1}{2}\big).$$

Thus the stated bound holds with

$$\psi_V(t) := \begin{cases} \frac{2^k}{C_{m-k}}\widetilde{V}_{\mathrm{rad}}(0) & \text{when } t \leqslant \frac{1}{2},\\ \frac{2^k}{C_{m-k}}\widetilde{V}_{\mathrm{rad}}\big(t-\frac{1}{2}\big) & \text{when } t > \frac{1}{2},\end{cases}$$

and ψ_V satisfies the further stated properties. □

Finally, we turn our attention to bounding integrals of functions concentrated near to a manifold Γ. In the case that Γ is a closed set and the function takes a simple form, a bound for the integral is immediate. Specifically, applying a spherical change of coordinates to $N_t^{\boldsymbol{u}}$ to give $\mu_{m-k}(\mathrm{d}\boldsymbol{n}) = \lambda^{m-k-1}\,\mathrm{d}\lambda\,\mu_{m-k-1}(\mathrm{d}\hat{\boldsymbol{n}})$, we have

$$\begin{aligned}&\left|\int_{\mathrm{tub}_t(\Gamma)} a(\mathrm{near}(\boldsymbol{z},\Gamma))\psi(\mathrm{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z}\right|\\ &\quad= \left|\int_\Gamma\int_{\widehat{N}^{\boldsymbol{u}}}\int_{[0,t]} a(\boldsymbol{u})\psi(\lambda)\det(I-S^{\boldsymbol{u}}(\lambda\hat{\boldsymbol{n}}))\,\lambda^{m-k-1}\,\mathrm{d}\lambda\,\mu_{m-k-1}(\mathrm{d}\hat{\boldsymbol{n}})\mu_k(\mathrm{d}\boldsymbol{u})\right|\\ &\quad\leqslant \big(\tfrac{3}{2}\big)^k\mu_{m-k-1}(\mathbb{S}^{m-k-1})\|a\|_{L^1(\Gamma)}\|\lambda^{m-k-1}\psi(\lambda)\|_{L^1([0,t])}.\end{aligned}$$

The first result we cover does not have the assumption that Γ is closed, but the integrand does depend on $\operatorname{dist}(\boldsymbol{z},\Gamma)$ even outside of $\operatorname{tub}(\Gamma)$. However, we are able to make the integral tractable with the assumption that Γ is extensible and making use of Lemma 4.5.8 (and Remark 4.5.9). Since (by definition) such sets are always bounded, we do not attempt to include any dependence on position in Γ in the integrand; such a factor could be dealt with by bounding it by its supremum. The result also applies to any closed bounded C^2 manifold, since those are C^2 extensible with $\Gamma^{(\mathrm{o})} = \operatorname{ext}_t(\Gamma) = \Gamma$.

Lemma 4.6.7. *Let Γ be a C^2 extensible set, let $s > 0$ such that the conclusion of Theorem 4.5.7 holds with $\tau = 2s$ (i.e. $\operatorname{tub}_{2s}(\operatorname{ext}_{2s}(\Gamma))$ is a tubular neighbourhood) and such that the conclusion of Lemma 4.5.8 holds (in particular, $B_s(\Gamma) \subseteq \operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$). Let ψ be a decreasing function with $\operatorname{supp}\psi \subseteq [0,s]$. Then*

$$\int_{\mathbb{R}^m} \psi(\operatorname{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z} \leqslant \left(\tfrac{3}{2}\right)^k \mu_{m-k-1}(\mathbb{S}^{m-k-1})\,\mu_k(\operatorname{ext}_{2s}(\Gamma)) \int_0^s \lambda^{m-k-1}\psi(\lambda)\,\mathrm{d}\lambda.$$

Proof. The support of $\psi(\operatorname{dist}(\boldsymbol{z},\Gamma))$ is contained in $B_s(\Gamma)$, which is contained in $\operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))$, so

$$\int_{\mathbb{R}^m} \psi(\operatorname{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z} = \int_{\operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))} \psi(\operatorname{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z} \leqslant \int_{\operatorname{tub}_s(\operatorname{ext}_{2s}(\Gamma))} \psi\left(\left|(e^{-1}(\boldsymbol{z}))_2\right|\right)\mathrm{d}\boldsymbol{z}.$$

By Lemma 4.3.3 this implies that

$$\int_{\mathbb{R}^m} \psi(\operatorname{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z} \leqslant \int_{\operatorname{ext}_{2s}(\Gamma)} \int_{N_s^{\boldsymbol{u}}} \psi(|\boldsymbol{n}|)\det(I - S^{\boldsymbol{u}}(\boldsymbol{n}))\,\mu_{m-k}(\mathrm{d}\boldsymbol{n})\,\mu_k(\mathrm{d}\boldsymbol{u}).$$

Now denote $\widehat{N}^{\boldsymbol{u}} := \{\hat{\boldsymbol{n}} \in N^{\boldsymbol{u}} : |\hat{\boldsymbol{n}}| = 1\}$ and use a spherical change of coordinates; this becomes

$$\int_{\mathbb{R}^m} \psi(\operatorname{dist}(\boldsymbol{z},\Gamma))\,\mathrm{d}\boldsymbol{z} \leqslant \int_{\operatorname{ext}_{2s}(\Gamma)} \int_{\widehat{N}^{\boldsymbol{u}}} \int_{[0,s]} \psi(\lambda)\det(I - S^{\boldsymbol{u}}(\lambda\hat{\boldsymbol{n}}))\,\lambda^{m-d-1}\,\mathrm{d}\lambda\,\mu_{m-k-1}(\mathrm{d}\hat{\boldsymbol{n}})\,\mu_k(\mathrm{d}\boldsymbol{u}).$$

Now the result follows from Lemma 4.6.1. □

The final result of this section bounds integrals of functions concentrated near to a codimension 1 manifold Γ. Unlike the previous result, we cannot just bound the factor a that varies along Γ by its supremum because Γ can be unbounded, in which case we will need to use the decay of a to show that the integral is finite. In fact we could take the supremum of a only in the normal direction, which gives a bound like

$$\sup_{\lambda\in(-t,t)} \int_\Gamma |a(\boldsymbol{u} + \lambda\boldsymbol{n}(\boldsymbol{u}))|\,\mu_{m-1}(\mathrm{d}\boldsymbol{u}).$$

There is no technical reason not to use a bound like this for the first inequality, but this is a rather awkward expression, so we use Taylor's theorem in the normal direction to obtain bounds in terms of the L^1 norms of a and its derivatives. In the second inequality we are integrating the difference between $a(\boldsymbol{z})$ and $a(\boldsymbol{u})$, so some use of Taylor's theorem in the normal direction really is essential, but we use an extra term to obtain a convenient expression. The third, rather different-looking, inequality is a useful side effect of doing this computation; it shows that if a and its derivatives are integrable on $\mathbb{R}^m$ and Γ has a tubular neighbourhood then a is integrable on Γ.

Lemma 4.6.8. *Let $\Gamma \subseteq \mathbb{R}^m$ and $s > 0$ satisfy one of the following:*

- *Let Γ be an orientable C^2 manifold of dimension $m-1$ that is closed (but possibly unbounded) with $\tau(\Gamma) > 0$. Let $s \leqslant \frac{1}{2}\tau(\Gamma)$.*
- *Let Γ be an orientable C^2 extensible manifold of dimension $m-1$. Let s be sufficiently small that $\mathrm{tub}_{2s}(\Gamma)$ is a tubular neighbourhood and the conclusion of Lemma 4.5.8 holds (so that we may write the distance function and nearest point function in terms of e).*

Denote $\delta(\boldsymbol{z}) := \mathrm{dist}(\boldsymbol{z}, \Gamma)$ and $\boldsymbol{u}(\boldsymbol{z}) := \mathrm{near}(\boldsymbol{z}, \Gamma)$. Then

$$\int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{z})\psi(\delta(\boldsymbol{z}))| \,\mathrm{d}\boldsymbol{z} \leqslant 2\Big(\big(\tfrac{3}{2}\big)^{m-1} \|a\|_{L^1(\Gamma)} + 3^{m-1} \|\nabla a\|_{L^1(\mathbb{R}^m)}\Big) \int_0^s \psi(\lambda)\,\mathrm{d}\lambda,$$

$$\int_{\mathrm{tub}_s(\Gamma)} \Big|\big(a(\boldsymbol{z}) - a(\boldsymbol{u}(\boldsymbol{z}))\big)\psi(\delta(\boldsymbol{z}))\Big| \,\mathrm{d}\boldsymbol{z} \leqslant 2\Big(\big(\tfrac{3}{2}\big)^{m-1} \|\nabla a\|_{L^1(\Gamma)} + 3^{m-1} \|\nabla \otimes \nabla a\|_{L^1(\mathbb{R}^m)}\Big) \int_0^s \lambda\psi(\lambda)\,\mathrm{d}\lambda,$$

and furthermore

$$\int_\Gamma |a(\boldsymbol{u})| \,\mathrm{d}\boldsymbol{u} \leqslant \frac{2^{m-2}}{s} \|a\|_{L^1(\mathbb{R}^m)} + 6^{m-1} \|\nabla a\|_{L^1(\mathbb{R}^m)}.$$

Proof. First and third inequality. We will first bound another integral. Using Remark 4.2.5 or Remark 4.5.9, we have

$$\int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{z}) - a(\boldsymbol{u}(\boldsymbol{z}))| \psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} = \int_\Gamma \int_{-s}^{s} |a(\boldsymbol{u} + \lambda \boldsymbol{n}(\boldsymbol{u})) - a(\boldsymbol{u})| \psi(|\lambda|) \det(I_k - \lambda S^{\boldsymbol{u}})\,\mathrm{d}\lambda\, \mu_k(\mathrm{d}\boldsymbol{u}).$$

We will apply Taylor's theorem to a in the $\boldsymbol{n}(\boldsymbol{u})$ direction with one term, which says

$$a(\boldsymbol{u} + \lambda \boldsymbol{n}(\boldsymbol{u})) - a(\boldsymbol{u}) = \int_0^1 \lambda(\boldsymbol{n}(\boldsymbol{u}) \cdot \nabla) a(\boldsymbol{u} + t\lambda \boldsymbol{n}(\boldsymbol{u}))\,\mathrm{d}t.$$

Substituting this in and changing variables $t' = t\lambda$ we obtain

$$\begin{aligned}
&\int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{z}) - a(\boldsymbol{u}(\boldsymbol{z}))| \psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} \\
&\quad \leqslant \int_\Gamma \int_{-s}^{s} \int_0^1 |\lambda(\boldsymbol{n}(\boldsymbol{u}) \cdot \nabla) a(\boldsymbol{u} + t\lambda \boldsymbol{n}(\boldsymbol{u})) \psi(|\lambda|) \det(I_k - \lambda S^{\boldsymbol{u}})|\,\mathrm{d}t\,\mathrm{d}\lambda\, \mu_{m-1}(\mathrm{d}\boldsymbol{u}) \\
&\quad \leqslant \left(\frac{3}{2}\right)^{m-1} \int_\Gamma \int_{-s}^{s} \int_{[0,\lambda]} |\nabla a(\boldsymbol{u} + t' \boldsymbol{n}(\boldsymbol{u}))| \psi(|\lambda|)\,\mathrm{d}t'\,\mathrm{d}\lambda\, \mu_{m-1}(\mathrm{d}\boldsymbol{u}) \\
&\quad \leqslant 3^{m-1} \int_\Gamma \int_{-s}^{s} \int_{-s}^{s} |\nabla a(\boldsymbol{u} + t' \boldsymbol{n}(\boldsymbol{u}))| \psi(|\lambda|) \det(I + t' S^{\boldsymbol{u}})\,\mathrm{d}t'\,\mathrm{d}\lambda\, \mu_{m-1}(\mathrm{d}\boldsymbol{u}) \\
&\quad = 2 \times 3^{m-1} \int_{\mathrm{tub}_s(\Gamma)} |\nabla a(\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y} \int_0^s \psi(\lambda)\,\mathrm{d}\lambda.
\end{aligned}$$

We now obtain the first inequality by using this bound in

$$\int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{z})| \psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} \leqslant \int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{u}(\boldsymbol{z}))| \psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} + \int_{\mathrm{tub}_s(\Gamma)} |a(\boldsymbol{z}) - a(\boldsymbol{u}(\boldsymbol{z}))| \psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z},$$

and using Lemma 4.6.1 for the first term. For the final inequality note that

$$\int_{\Gamma}|a(\boldsymbol{u})|\,\mu_{m-1}(\mathrm{d}\boldsymbol{u}) = \frac{1}{2s}\int_{\Gamma}\int_{-s}^{s}|a(\boldsymbol{u})|\,\mathrm{d}\lambda\,\mu_{m-1}(\mathrm{d}\boldsymbol{u}) \leqslant \frac{2^{m-1}}{2s}\int_{\mathrm{tub}_s(\Gamma)}|a(\boldsymbol{u}(\boldsymbol{z}))|\,\mathrm{d}\boldsymbol{z}$$
$$\leqslant \frac{2^{m-1}}{2s}\int_{\mathrm{tub}_s(\Gamma)}|a(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} + \frac{2^{m-1}}{2s}\int_{\mathrm{tub}_s(\Gamma)}|a(\boldsymbol{z})-a(\boldsymbol{u}(\boldsymbol{z}))|\,\mathrm{d}\boldsymbol{z},$$

and use the above bound for the second term with $\psi \equiv 1$ (so that $\int_0^s \psi(\lambda)\,\mathrm{d}\lambda = s$).

Second inequality. This is proved in exactly the same way as the first inequality, but using one more term in Taylor's theorem. The integral is

$$\int_{\mathrm{tub}_s(\Gamma)}|a(\boldsymbol{z})-a(\boldsymbol{u}(\boldsymbol{z}))|\psi(\delta(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} = \int_{\Gamma}\int_{-s}^{s}\Big(a(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))-a(\boldsymbol{u})\Big)\psi(|\lambda|)\det(I_k-\lambda S^{\boldsymbol{u}})\,\mathrm{d}\lambda\,\mu_k(\mathrm{d}\boldsymbol{u}),$$

and Taylor's theorem says that

$$a(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))-a(\boldsymbol{u}) = \lambda\boldsymbol{n}(\boldsymbol{u})\cdot\nabla a(\boldsymbol{u}) + \int_0^1(1-t)\lambda^2(\boldsymbol{n}(\boldsymbol{u})\cdot\nabla)^2 a(\boldsymbol{u}+t\lambda\boldsymbol{n}(\boldsymbol{u}))\,\mathrm{d}t.$$

The first term is thus bounded by

$$\left(\frac{3}{2}\right)^{m-1}\int_{\Gamma}\int_{-s}^{s}|\boldsymbol{n}(\boldsymbol{u})\cdot\nabla a(\boldsymbol{u})|\,|\lambda|\psi(|\lambda|)\,\mathrm{d}\lambda\,\mu_k(\mathrm{d}\boldsymbol{u}) \leqslant 2\left(\tfrac{3}{2}\right)^{m-1}\|\nabla a\|_{L^1(\Gamma)}\int_0^s \lambda\psi(\lambda)\,\mathrm{d}\lambda.$$

Again change variables $t' = t\lambda$ for the second term, so that

$$\left|\int_{\Gamma}\int_{-s}^{s}\int_0^1(1-t)\lambda^2(\boldsymbol{n}(\boldsymbol{u})\cdot\nabla)^2 a(\boldsymbol{u}+t\lambda\boldsymbol{n}(\boldsymbol{u}))\psi(|\lambda|)\det(I_k-\lambda S^{\boldsymbol{u}})\,\mathrm{d}t\,\mathrm{d}\lambda\,\mu_{m-1}(\mathrm{d}\boldsymbol{u})\right|$$
$$\leqslant \left(\frac{3}{2}\right)^{m-1}\int_{\Gamma}\int_{-s}^{s}\int_{[0,\lambda]}|\nabla\otimes\nabla a(\boldsymbol{u}+t'\boldsymbol{n}(\boldsymbol{u}))|\,|\lambda|\psi(|\lambda|)\,\mathrm{d}t'\,\mathrm{d}\lambda\,\mu_{m-1}(\mathrm{d}\boldsymbol{u})$$
$$\leqslant 3^{m-1}\int_{\Gamma}\int_{-s}^{s}\int_{-s}^{s}|\nabla\otimes\nabla a(\boldsymbol{u}+t'\boldsymbol{n}(\boldsymbol{u}))|\,|\lambda|\psi(|\lambda|)\det(I+t'S^{\boldsymbol{u}})\,\mathrm{d}t'\,\mathrm{d}\lambda\,\mu_{m-1}(\mathrm{d}\boldsymbol{u})$$
$$\leqslant 2\times 3^{m-1}\int_{\mathrm{tub}_s(\Gamma)}|\nabla\otimes\nabla a(\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y}\,\sup_{\boldsymbol{u}\in\Gamma}\int_0^s\psi(\lambda)\,\mathrm{d}\lambda. \qquad \square$$

Chapter 5

Statement of result

In this chapter we state the main result of this thesis: a two-term Szegő theorem for generalised anti-Wick operators. In fact, as discussed in §1.5, we will prove the theorem for the even more general class of operators of the form

$$T_r[p] := \mathrm{op}[W * p_r], \qquad \text{where for } \boldsymbol{z} \in \mathbb{R}^{2d} \text{ we set } p_r(\boldsymbol{z}) := p(\boldsymbol{z}/r).$$

In §5.1 the basic properties of operators of this form are given. In §5.2 we precisely state the result: the asymptotic formula

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^{2d} A_0(a, \Omega, f) + r^{2d-1} A_1(a, \Omega, f; W) + O(r^{2d-2}),$$

where the asymptotic terms A_0 and A_1 are defined in that section. The result is only for sufficiently smooth f, but in §5.3 we use an approximation argument to show that it also holds for certain indicator functions, which gives information about the eigenvalue counting function.

In §5.4 we relate the statement of the Szegő theorem and eigenvalue counting function corollary to generalised anti-Wick operators: the conditions on W and expression of A_1 in terms of W are rephrased in terms of the window functions. We also recall simple sufficient conditions for generalised anti-Wick operators to be positive, which gives a form of the Szegő theorem for $f(t) = \log(1+t)$. Some particularly common special cases of generalised anti-Wick operators, for which the convolution factor W is spherically symmetric, are discussed in §5.5.

In §5.6, for a class of examples where $\partial\Omega$ contains a cusp (with $d = 1$ and $f(t) = t^2$), we show

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^2 A_0(a, \Omega, f) + r A_1(a, \Omega, f; W) + \Theta\big(r\,\omega^{-1}(1/r)\big).$$

The remainder $\Theta\big(r\,\omega^{-1}(1/r)\big)$, which is explained in that section, is larger than in the main theorem, so this shows that the conclusion of the main result does not hold if the conditions are relaxed to include to include these examples.

§5.7 describes the idea of the proof of the theorem. (The full proof is given later, in Chapter 6.) Finally, §5.8 contains some basic technical results about the boundary term A_1.

5.1 Basic properties of the operator

As stated in the introduction, the operators of interest here depend on a discontinuous symbol p dilated by a factor r and convolved with a Schwartz function $W \in \mathscr{S}(\mathbb{R}^{2d})$. The dependence on W will not be the focus of most of the proof, so we suppress that from the notation:

Notation 5.1.1. For a Schwartz function $W \in \mathscr{S}(\mathbb{R}^{2d})$ whose integral equals 1, for $p \in L^{\infty}(\mathbb{R}^{2d})$ and for each $r > 0$, we denote

$$T_r[p] := \mathrm{op}[W * p_r], \qquad \text{where for } \boldsymbol{z} \in \mathbb{R}^{2d} \text{ we set } p_r(\boldsymbol{z}) := p(\boldsymbol{z}/r).$$

In this section we prove a few basic properties of this operator. The presence of the convolution in the symbol means that we will repeatedly need basic properties of convolution.

Lemma 5.1.2. *If $a \in L^1(\mathbb{R}^m)$ and $b \in L^p(\mathbb{R}^m)$ for $1 \leqslant p \leqslant \infty$ then*

$$\|a * b\|_{L^p} \leqslant \|a\|_{L^1}\|b\|_{L^p}.$$

If $a, b \in L^1(\mathbb{R}^m)$ then

$$\int a * b(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int a(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \int b(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

If $a \in L^{\infty}(\mathbb{R}^m)$, $b \in L^1(\mathbb{R}^m)$, and the j^{th} derivative of a exists with $\partial_j a \in L^{\infty}(\mathbb{R}^m)$ then $\partial_j(a * b)$ exists and satisfies

$$\partial_j(a * b) = (\partial_j a) * b.$$

Proof. These are standard facts. The first is a simple special case of Young's inequality (see Lang, 1993, Chapter XIII, Theorem 1.2). When $p = 1$ this allows us to apply Fubini's theorem to the integral of $a * b$, which proves the second fact. The final one is a matter of differentiating under the integral, which the stated conditions permit (see Lang, 1993, Chapter XIII, Lemma 2.2). □

Combining the above lemma with the standard norm bounds and trace formula for Weyl symbols, we arrive at the analogous results for $T_r[p]$.

Lemma 5.1.3. *Let $p \in L^{\infty}(\mathbb{R}^{2d}) \cap L^1(\mathbb{R}^{2d})$. Then the operator norm and trace norm of $T_r[p]$ satisfy*

$$\|T_r[p]\| \leqslant C_d \sum_{|\boldsymbol{k}| \leqslant d+2} \|\partial^{\boldsymbol{k}} W\|_{L^1(\mathbb{R}^{2d})} \|p\|_{L^{\infty}(\mathbb{R}^{2d})},$$
$$\|T_r[p]\|_1 \leqslant C'_d r^{2d} \sum_{|\boldsymbol{k}| \leqslant 2d+1} \|\partial^{\boldsymbol{k}} W\|_{L^1(\mathbb{R}^{2d})} \|p\|_{L^1(\mathbb{R}^{2d})}.$$

This implies that $T_r[p]$ is trace class, with trace given by

$$\operatorname{tr} T_r[p] = \frac{r^{2d}}{(2\pi)^d} \int_{\mathbb{R}^{2d}} p(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}.$$

Proof. By Lemma 5.1.2 we have $\partial^{\boldsymbol{k}}(W * p_r) = (\partial^{\boldsymbol{k}} W) * p_r$, and

$$\|(\partial^{\boldsymbol{k}} W) * p_r\|_{L^\infty} \leqslant \|\partial^{\boldsymbol{k}} W\|_{L^1} \|p_r\|_{L^\infty} = \|\partial^{\boldsymbol{k}} W\|_{L^1} \|p\|_{L^\infty},$$
$$\|(\partial^{\boldsymbol{k}} W) * p_r\|_{L^1} \leqslant \|\partial^{\boldsymbol{k}} W\|_{L^1} \|p_r\|_{L^1} = r^{2d} \|\partial^{\boldsymbol{k}} W\|_{L^1} \|p\|_{L^1},$$

so Lemma 2.1.2 and Lemma 2.1.3 imply the stated bounds. The trace is then

$$\begin{aligned}
\operatorname{tr} T_r[p] &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} W * p_r(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z} \\
&= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z} \int_{\mathbb{R}^{2d}} p\left(\frac{\boldsymbol{z}}{r}\right) \mathrm{d}\boldsymbol{z} \\
&= \frac{r^{2d}}{(2\pi)^d} \int_{\mathbb{R}^{2d}} p(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z}. \qquad \square
\end{aligned}$$

Notation 5.1.4. Since we will be interested in the effects of varying the scale of the discontinuous part of the symbol, rather than varying W, we will often use the notation

$$x \lesssim y \qquad \Longleftrightarrow \qquad \text{there exists } C_W > 0 \text{ such that } x \leqslant C_W \, y,$$

where C_W is some constant depending only on W and the dimension d (not on p or r). For example, with this notation the above lemma says that

$$\|T_r[p]\| \lesssim \|p\|_{L^\infty(\mathbb{R}^{2d})}, \qquad \|T_r[p]\|_1 \lesssim r^{2d} \|p\|_{L^1(\mathbb{R}^{2d})}.$$

Finally, we will often work with $f(T_r[p])$ where $f(0) = 0$; indeed the main result of this thesis is a statement about the trace of this operator. It is therefore important that it is a trace class operator. In the self-adjoint case this will follow from writing $f(t) = t g(t)$ where g is sufficiently regular, as expressed in the next lemma.

Lemma 5.1.5. *Let $f \in C^\infty(\mathbb{R})$ such that $f(0) = 0$. Set*

$$g(t) := \begin{cases} f(t)/t & \text{when } t \neq 0, \\ f'(0) & \text{when } t = 0. \end{cases}$$

Then $g \in C^\infty(\mathbb{R})$, and for each $t \in \mathbb{R}$ and $n \in \mathbb{N}_0$ we have

$$|\partial^n g(t)| \leqslant \frac{1}{n+1} \sup_{s \in [0,t]} |\partial^{n+1} f(s)|;$$

in particular,

$$|f(t)| \leqslant |t| \sup_{s \in [0,t]} |f'(s)|.$$

Proof. We first observe that g satisfies

$$g(t) = \int_0^1 f'(tx) \, \mathrm{d}x.$$

This is immediate for $t = 0$. For $t \neq 0$ it follows from the fact that

$$f(t) = \int_0^t f'(y)\,\mathrm{d}y = t\int_0^1 f'(tx)\,\mathrm{d}x.$$

We may differentiate under the integral in this representation of g, so that

$$\partial^n g(t) = \int_0^1 x^n \partial^{n+1} f(tx)\,\mathrm{d}x;$$

bounding $\partial^{n+1} f$ by its supremum and evaluating the integral gives the stated bound on $|\partial^n g(t)|$. The final inequality follows from this with $n = 0$ by writing $f(t) = t g(t)$ (or by applying the mean value theorem to $f(t) - f(0)$). □

We are now in a position to prove that $f(T_r[p])$ is trace class.

Lemma 5.1.6. *Let A be a trace class (and therefore bounded) operator on $L^2(\mathbb{R}^d)$, and let f be a function satisfying $f(0) = 0$ and one of the following two conditions:*

- *Let f be an analytic function on $\mathbb{C}$ (i.e. have infinite radius of convergence).*
- *Let $f \in C^\infty(\mathbb{R})$, and let A be self-adjoint.*

Then $f(A)$ is a trace class operator.

In the case that $A = T_r[p]$, note that a sufficient condition for A to be self-adjoint is that W and p be real-valued, because this ensures that the Weyl symbol of A is real-valued.

Proof. The complex-analytic case is immediate from Lemma 3.3.1 (which includes an explicit bound on the trace norm of $f(A)$). For the self-adjoint case, we use Lemma 5.1.5 to write

$$f(A) = A g(A).$$

Thus

$$\|f(A)\|_1 \leqslant \|A\|_1 \|g(A)\| \leqslant \|A\|_1 \sup_{|t| \leqslant \|A\|} |g(t)| \leqslant \|A\|_1 \sup_{|t|\leqslant\|A\|} |f'(t)|.$$ □

5.2 Szegő theorem

In this section we state the main result of this thesis: a Szegő theorem for operators of the form $T_r[a\chi_\Omega]$. This is Theorem 5.2.6 when the boundary of Ω is C^2, and Theorem 5.2.8 when it is piecewise C^2. The first form of the result is not strictly contained in the second because Theorem 5.2.8 contains the additional hypothesis that Ω is compact. In the case of generalised anti-Wick operators, the conditions and conclusions can be explicitly expressed in terms of the windows instead of W; see §5.4.

The result is that, for suitable symbols, as $r \to \infty$ we have

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^{2d} A_0(a, \Omega, f) + r^{2d-1} A_1(a, \Omega, f; W) + O(r^{2d-2}).$$

The boundary term A_1 depends on a type of directional antiderivative of W. Specifically, for any $W \in \mathscr{S}(\mathbb{R}^{2d})$ with $\int_{\mathbb{R}^{2d}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, we define

$$Q_{\boldsymbol{\omega}}(\lambda) := \int_{\{\boldsymbol{z}\in\mathbb{R}^{2d}:\boldsymbol{z}\cdot\boldsymbol{\omega}\leqslant\lambda\}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \qquad (\boldsymbol{\omega}\in\mathbb{S}^{2d-1}).$$

This satisfies $\lim_{\lambda\to\infty} Q_{\boldsymbol{\omega}}(\lambda) = \int_{\mathbb{R}^{2d}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, and so

$$1 - Q_{\boldsymbol{\omega}}(\lambda) = \int_{\{\boldsymbol{z}\in\mathbb{R}^{2d}:\boldsymbol{z}\cdot\boldsymbol{\omega}\geqslant\lambda\}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \qquad (\boldsymbol{\omega}\in\mathbb{S}^{2d-1}).$$

Notation 5.2.1. The asymptotic terms are

$$\begin{aligned} A_0(a,\Omega,f) &= \frac{1}{(2\pi)^d}\int_\Omega f(a(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z}, \\ A_1(a,\Omega,f;W) &= \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}\Big(f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)a(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(a(\boldsymbol{u}))\Big)\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}). \end{aligned}$$

Remark 5.2.2. When $a \in L^1(\Omega)$ and $a \in L^1(\partial\Omega)$ these expressions are well defined. Indeed, using Lemma 5.1.5 we see that A_0 satisfies

$$|A_0(a,\Omega,f)| \leqslant \frac{1}{(2\pi)^d}\|a\|_{L^1(\Omega)} \sup_{|t|\leqslant\|a\|_{L^\infty(\Omega)}} |f'(t)|.$$

A bound for the second term is given in Lemma 5.8.2.

We need a condition on the regularity of f. It depends on whether we define $f(T_r[a\chi_\Omega])$ using the holomorphic functional calculus or the Borel functional calculus. In the latter case we impose additional restrictions on W and a to ensure that the operator $T_r[a\chi_\Omega]$ is self-adjoint (by ensuring that its Weyl symbol is real).

Condition 5.2.3. For functions a and W, let f be a function satisfying $f(0) = 0$ and one of the following.

1. Let f be an analytic function on $\mathbb{C}$.
2. Let a be real-valued, let W be real-valued and let $f \in C^\infty(\mathbb{R})$.

The C^2 boundary form of the theorem has the following regularity conditions on the symbol.

Condition 5.2.4. Let both of the following be satisfied.

- Let $\Omega \subseteq \mathbb{R}^{2d}$ be a C^2 domain such that $\partial\Omega$ has a tubular neighbourhood (see §4.2).
- Let $a \in C^2(\mathbb{R}^{2d})$ satisfying $\partial^{\boldsymbol{k}} a \in L^1(\mathbb{R}^{2d}) \cap L^\infty(\mathbb{R}^{2d})$ for all $\boldsymbol{k} \in \mathbb{N}_0^{2d}$ such that $|\boldsymbol{k}| \leqslant 2$.

Remark 5.2.5. Whenever Condition 5.2.4 is satisfied we can conclude that that a satisfies the boundary integrability properties $\partial^{\boldsymbol{k}} a \in L^1(\partial\Omega)$ for $|\boldsymbol{k}| \leqslant 1$. This fact is the third inequality in Lemma 4.6.8.

Theorem 5.2.6. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ satisfy $\int_{\mathbb{R}^{2d}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$. Let W, a, Ω, f satisfy Condition 5.2.3 and Condition 5.2.4. Then*

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^{2d} A_0(a,\Omega,f) + r^{2d-1} A_1(a,\Omega,f;W) + O(r^{2d-2})$$

as $r \to \infty$.

The idea behind the proof is discussed in §5.7, and the full proof is given in Chapter 6, specifically in §6.1 and §6.2.

We now turn our attention to the second form of the result, where we allow the boundary of Ω to have "corners". Roughly speaking we require that $\partial\Omega$ is piecewise C^2, but the condition is slightly stronger: each piece must be strongly extensible, a concept defined in §4.5, and the set of "corners" of codimension 2 is also piecewise C^2 extensible. We also demand that the particular way that $\partial\Omega$ is expressed as a union of smaller sets is not too redundant in terms of overlapping pieces.

Condition 5.2.7. Let $\Omega \subseteq \mathbb{R}^m$ be a closed connected Lipschitz domain (see Definition 4.1.4), for which the boundary $\partial\Omega$ can be expressed as the union of a finite number of sets, that is,

$$\partial\Omega = \bigcup_{i\in I} \Gamma_i,$$

where I is a finite indexing set, and these sets satisfy both of the following:

- Each Γ_i is strongly C^2 extensible of dimension $m-1$, and for $i \neq j$ we have $\Gamma_i^{(\mathrm{i})} \cap \Gamma_j^{(\mathrm{i})} = \emptyset$.
- Denoting $\partial^2\Omega := \bigcup_{i\in I} \Gamma_i \setminus \Gamma_i^{(\mathrm{i})}$, we have that $\partial^2\Omega$ is itself the union of a finite number of sets (possibly zero), each of which is C^2 extensible of dimension $m-2$.

If Ω satisfies Condition 5.2.7 then the way of dividing $\partial\Omega$ into pieces is certainly not unique. For example, if Ω is the unit ball then we could consider $\partial\Omega$ as a single piece, or we could divide it into two hemispherical shells, in which case $\partial^2\Omega$ is a circle, which is C^2 extensible of dimension $m-2$. Of course, if $\partial\Omega$ can be expressed in the way demanded by Condition 5.2.7 then it can also be expressed as a union of sets that do not satisfy it; the condition just demands that at least one such representation exists.

We may now state the form of the main result for non-smooth domains.

Theorem 5.2.8. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ with $\int W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, let Ω satisfy Condition 5.2.7 with $m = 2d$, let $a \in C^2(\Omega)$, and let W, a, f satisfy Condition 5.2.3. Then*

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^{2d} A_0(a,\Omega,f) + r^{2d-1} A_1(a,\Omega,f;W) + O(r^{2d-2})$$

as $r \to \infty$.

The idea behind the proof of this part is also discussed in §5.7, and the full proof is given in Chapter 6, specifically in §6.4 and §6.5.

5.3 Eigenvalue counting function

As discussed in Chapter 1, one application of Szegő theorems is that, by setting the function of the operator to an indicator function χ_I, the result concerns $\operatorname{tr}\chi_I(T)$, which is the number of eigenvalues of T in the set I. We cannot directly apply the Szegő theorem for $T_r[a\chi_\Omega]$ with $f=\chi_I$ because this function is not sufficiently smooth to satisfy Condition 5.2.3, but we may still obtain an eigenvalue counting result with a standard approximation argument, which is detailed in this section. We use the notation $N(T_r[\chi_\Omega],[\delta,\infty))$ to mean the number of eigenvalues of $T_r[\chi_\Omega]$ in the interval $[\delta,\infty)$.

Corollary 5.3.1. *Let $\Omega\subseteq\mathbb{R}^{2d}$ satisfy Condition 5.2.7. Let $W\in\mathscr{S}(\mathbb{R}^{2d})$ be real-valued and satisfy $\int_{\mathbb{R}^{2d}} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}=1$. Let $\delta\in(0,1)$ such that*

$$\forall\boldsymbol{\omega}\in\mathbb{S}^{2d-1} \text{ we have } \mu_1(\{\lambda\in\mathbb{R}:Q_{\boldsymbol{\omega}}(\lambda)=\delta\})=0.$$

Then

$$N(T_r[\chi_\Omega],[\delta,\infty))=r^{2d}A_0(1,\Omega,\chi_{[\delta,\infty)})+r^{2d-1}A_1(1,\Omega,\chi_{[\delta,\infty)};W)+o(r^{2d-1})$$

as $r\to\infty$. Specifically, these terms satisfy

$$A_0(1,\Omega,\chi_{[\delta,\infty)})=\frac{1}{(2\pi)^d}\mu_{2d}(\Omega),$$
$$A_1(1,\Omega,\chi_{[\delta,\infty)};W)=\frac{1}{(2\pi)^d}\int_{\partial\Omega}g_{\boldsymbol{n}(\boldsymbol{u})}(\delta)\mu_{2d-1}(\mathrm{d}\boldsymbol{u}),$$

where for each $\delta\in(0,1)$, $\boldsymbol{\omega}\in\mathbb{S}^{2d-1}$ we set

$$g_{\boldsymbol{\omega}}(\delta):=\mu_1(\{\lambda\in(-\infty,0]:Q_{\boldsymbol{\omega}}(\lambda)>\delta\})-\mu_1(\{\lambda\in[0,\infty):Q_{\boldsymbol{\omega}}(\lambda)<\delta\}).$$

Remark 5.3.2. The statement of Corollary 5.3.1 is somewhat simpler when $Q_{\boldsymbol{\omega}}$ is a non-decreasing function for all $\boldsymbol{\omega}\in\mathbb{S}^{2d-1}$. A sufficient condition for this is that W is non-negative, and another sufficient condition is that the operator is a generalised anti-Wick operator with $\varphi_1=\varphi_2$ (see Lemma 5.4.2). In this case:

- The condition relating $Q_{\boldsymbol{\omega}}$ and δ holds if and only if for each $\boldsymbol{\omega}\in\mathbb{S}^{2d-1}$ there exists a unique $\lambda\in\mathbb{R}$ such that $Q_{\boldsymbol{\omega}}(\lambda)=\delta$; we denote such a λ by $Q_{\boldsymbol{\omega}}^{-1}(\delta)$, even if $Q_{\boldsymbol{\omega}}$ is not invertible on its whole domain.

- We then have $g_{\boldsymbol{\omega}}(\delta)=-Q_{\boldsymbol{\omega}}^{-1}(\delta)$, so the boundary term simplifies to

$$A_1(1,\Omega,\chi_{[\delta,\infty)};W)=-\frac{1}{(2\pi)^d}\int_{\partial\Omega}Q_{\boldsymbol{n}(\boldsymbol{u})}^{-1}(\delta)\mu_{2d-1}(\mathrm{d}\boldsymbol{u}).$$

  This holds because, by Lemma 5.8.3, $A_1(1,\Omega,\chi_{[\delta,\infty)};W)$ is the integral over $\partial\Omega$ of

$$\int_{\mathbb{R}}\Big(\chi_{[\delta,\infty)}(Q_{\boldsymbol{\omega}}(\lambda))-\chi_{[0,\infty)}(\lambda)\Big)\mathrm{d}\lambda=\int_{Q_{\boldsymbol{\omega}}^{-1}(\delta)}^{0}\mathrm{d}\lambda=-Q_{\boldsymbol{\omega}}^{-1}(\delta).$$

Proof of Corollary 5.3.1. Let $\varepsilon > 0$. Let $f_{-\varepsilon}$ and $f_{+\varepsilon}$ be smooth increasing functions satisfying $f_{\pm\varepsilon}(t) = \chi_{[\delta,\infty)}(t)$ except when $t \in (\delta, \delta+\varepsilon)$ and $t \in (\delta-\varepsilon, \delta)$ respectively. These conditions imply that $0 \leqslant f_{-\varepsilon} \leqslant \chi_{[\delta,\infty)} \leqslant f_{+\varepsilon} \leqslant 1$, so

$$\operatorname{tr} f_{-\varepsilon}(T_r[\chi_\Omega]) \leqslant \operatorname{tr} \chi_{[\delta,\infty)}(T_r[\chi_\Omega]) \leqslant \operatorname{tr} f_{+\varepsilon}(T_r[\chi_\Omega]).$$

For $\varepsilon < \delta$ we have $f_\pm(0) = 0$. We now apply Theorem 5.2.8 to $f_{\pm\varepsilon}(T_r[\chi_\Omega])$ (with $a \equiv 1$). When $\varepsilon < 1-\delta$, the leading terms both satisfy

$$A_0(1, \Omega, f_{\pm\varepsilon}) = \frac{1}{(2\pi)^d} \int_\Omega f_{\pm\varepsilon}(1)\, \mathrm{d}\boldsymbol{z} = \frac{1}{(2\pi)^d} \mu_{2d}(\Omega),$$

so for all sufficiently small $\varepsilon > 0$ we have

$$\begin{aligned}
\lim_{r\to\infty} \frac{\operatorname{tr}\big((f_{+\varepsilon} - f_{-\varepsilon})(T_r[\chi_\Omega])\big)}{r^{2d-1}} &= \frac{1}{(2\pi)^d} \int_{\partial\Omega} \int_{\mathbb{R}} \Big(f_{+\varepsilon}(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)) - f_{-\varepsilon}(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)) \Big)\, \mathrm{d}\lambda\, \mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \\
&\leqslant \frac{1}{(2\pi)^d} \mu_{2d-1}(\partial\Omega) \sup_{\boldsymbol{u}\in\partial\Omega} \mu_1(\{\lambda \in \mathbb{R} : \delta - \varepsilon \leqslant Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) \leqslant \delta + \varepsilon\}).
\end{aligned}$$

The limit of this bound is 0 as $\varepsilon \to 0$, so the eigenvalue counting function satisfies the stated asymptotic form.

The expression for A_0 is immediate, and for A_1 note that by Lemma 5.8.3 we have

$$\begin{aligned}
&A_1(1, \Omega, \chi_{[\delta,\infty)}; W) \\
&\quad = \tilde{A}_1(1, \Omega, \chi_{[\delta,\infty)}; W) \\
&\quad = \frac{1}{(2\pi)^d} \int_{\partial\Omega} \int_{\mathbb{R}} \Big(\chi_{[\delta,\infty)}(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)) - \chi_{[0,\infty)}(\lambda) \Big)\, \mathrm{d}\lambda\, \mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \\
&\quad = \frac{1}{(2\pi)^d} \int_{\partial\Omega} \Big(\int_{-\infty}^0 \chi_{[\delta,\infty)}(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda))\, \mathrm{d}\lambda - \int_0^\infty \chi_{(-\infty,\delta)}(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda))\, \mathrm{d}\lambda \Big) \mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \\
&\quad = \frac{1}{(2\pi)^d} \int_{\partial\Omega} g_{\boldsymbol{n}(\boldsymbol{u})}(\delta)\, \mu_{2d-1}(\mathrm{d}\boldsymbol{u}). \qquad \square
\end{aligned}$$

5.4 Generalised anti-Wick operators

As discussed in §1.4 and §1.5, the main interest in operators of the form $T_r[a\chi_\Omega]$ is that they include, as a special case, generalised anti-Wick operators; that is, there exists a suitable W (depending on the windows) such that

$$T_r[p] = \mathscr{F}^*_{\varphi_2} p_r \mathscr{F}_{\varphi_1}, \qquad \text{where for } \boldsymbol{z} \in \mathbb{R}^{2d} \text{ we set } p_r(\boldsymbol{z}) := p(\boldsymbol{z}/r).$$

The Szegő theorem in §5.2 and its eigenvalue counting function corollary in §5.3 therefore apply to these operators. The three lemmas stated at the start of this section explain this relationship: the first says how all references to W in the conditions of the main result and corollary may be expressed in terms of the window functions, the second says that Remark 5.3.2 holds for these operators and in the one-dimensional case expresses $Q_{\boldsymbol{\omega}}$ in terms of the window function, and the third shows that for generalised anti-Wick operators we may apply the Szegő theorem with the function $f(t) = \log(1+t)$. After the statement of these three lemmas, we shall recall some standard properties of generalised anti-Wick operators, and the section finishes by using these properties to prove the lemmas.

The first lemma describes sufficient conditions for the Szegő theorem and corollary to hold.

Lemma 5.4.1. *Theorem 5.2.6, Theorem 5.2.8 and Corollary 5.3.1 hold for generalised anti-Wick operators, with the conditions on W replaced by requirements on the window functions as follows:*

- *For all the conditions on W in Theorem 5.2.6, Theorem 5.2.8 and Corollary 5.3.1 to hold (including that W is real-valued), it suffices that $\varphi_1 = \varphi_2$ (which we write simply as φ), $\varphi \in \mathscr{S}(\mathbb{R}^{2d})$, and $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$.*
- *For the conditions on W in Theorem 5.2.6 and Theorem 5.2.8 to hold <u>except</u> that W be real-valued (so we require Condition 5.2.3(1), the analytic f case), it suffices that $\varphi_1, \varphi_2 \in \mathscr{S}(\mathbb{R}^{2d})$ and $\langle \varphi_2, \varphi_1 \rangle_{L^2(\mathbb{R}^d)} = 1$.*

The proof is given later in this section. The next lemma is the observation that Remark 5.3.2 holds for generalised anti-Wick operators when the window functions are equal.

Lemma 5.4.2. *Let $\varphi \in \mathscr{S}(\mathbb{R}^m)$ with $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$. Then for each $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$, the function $Q_{\boldsymbol{\omega}}$ (corresponding to the generalised anti-Wick operator with the window φ) is non-decreasing.*

Again, the proof is given later in this section. In it, we find an explicit expression for $Q_{\boldsymbol{\omega}}$, even for generalised anti-Wick operators with $\varphi_1 \neq \varphi_2$, in terms of the fractional Fourier transform $\mathscr{F}^{\boldsymbol{\omega}}$ (which will be defined before the proof), which is of some interest in its own right. In one dimension this expression is

$$Q_{\boldsymbol{\omega}}(\lambda) = \int_{-\infty}^{\lambda} \mathscr{F}^{\boldsymbol{\omega}} \varphi_2(\eta) \overline{\mathscr{F}^{\boldsymbol{\omega}} \varphi_1(\eta)} \, \mathrm{d}\eta,$$

which immediately implies the lemma for $\varphi_1 = \varphi_2$ because the integrand is then non-negative. For higher dimensions the proof is similar, although the expression for $Q_{\boldsymbol{\omega}}$ in terms of component-wise fractional Fourier transforms is not quite as enlightening.

Just as with the early Szegő theorems for truncated Wiener–Hopf operators (see §1.2), a case of particular interest is $f(t) = \log(1+t)$ because

$$\operatorname{tr}\log(I + A) = \det(I + A).$$

The Szegő theorem in §5.2 does not include this case because $\log(1+t)$ is only defined on the interval $(-1, \infty)$. However, it does hold for this function for generalised anti-Wick operators, as this third lemma shows.

Lemma 5.4.3. *Let all of the following conditions hold:*

- *Let φ satisfy the first set of conditions in Lemma 5.4.1 (the self-adjoint case).*
- *Let $a \in C^2(\mathbb{R}^{2d})$ be real-valued and satisfy $a(\boldsymbol{z}) \geqslant c$ for all $\boldsymbol{z} \in \mathbb{R}^{2d}$, where $c > -1$.*
- *Let a and Ω satisfy Condition 5.2.4 (C^2 boundary case) or let Ω satisfy Condition 5.2.7 (compact with non-smooth boundary).*

Then

$$\operatorname{tr}\log(I + T_r[a\chi_\Omega]) = r^{2d} A_0(a, \Omega, \log(1+t)) + r^{2d-1} A_1(a, \Omega, \log(1+t); W) + O(r^{2d-2})$$

as $r \to \infty$.

The key fact that allows us to prove the results above is the connection between generalised anti-Wick operators and the Weyl quantisation, given by the following lemma.

Lemma 5.4.4. *Let $\varphi_1, \varphi_2 \in L^2(\mathbb{R}^d)$ and $p \in C_\mathrm{b}^\infty(\mathbb{R}^{2d})$. Then*

$$\mathscr{F}_{\varphi_2}^* p \mathscr{F}_{\varphi_1} = \operatorname{op}[\mathscr{W}_{\varphi_2,\varphi_1} * p], \qquad \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{x}, \xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}\boldsymbol{t}\cdot\xi} \varphi_2(\boldsymbol{x} + \tfrac{1}{2}\boldsymbol{t}) \overline{\varphi_1(\boldsymbol{x} - \tfrac{1}{2}\boldsymbol{t})} \,\mathrm{d}\boldsymbol{t}.$$

The function $\mathscr{W}_{\varphi_2,\varphi_1}$ is called the *Wigner transform* of φ_2, φ_1. This relationship can be found for example in Boggiatto, Cordero and Gröchenig (2004, Lemma 2.4), or when $\varphi_1 = \varphi_2$ in Folland (1989, Proposition (3.5)). These sources use a different convention from this thesis, so we now verify that this is the correct form.

Proof. Since our goal is simply to verify the correct scaling and multiplicative constants, we will work formally rather than showing that all relevant integrals converge. First note that for $u \in \mathscr{S}(\mathbb{R}^d)$ we have

$$\begin{aligned}\mathscr{F}_{\varphi_2}^* p \mathscr{F}_{\varphi_1} u(\boldsymbol{x}) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\xi} \mathrm{e}^{-\mathrm{i}\boldsymbol{y}\cdot\xi} u(\boldsymbol{y}) p(\boldsymbol{s}, \xi) \overline{\varphi_1(\boldsymbol{y} - \boldsymbol{s})} \varphi_2(\boldsymbol{x} - \boldsymbol{s}) \,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{s}\,\mathrm{d}\xi \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\boldsymbol{x}-\boldsymbol{y})\cdot\xi} b(\boldsymbol{x}, \boldsymbol{y}, \xi) u(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\xi,\end{aligned}$$

where

$$b(\boldsymbol{x}, \boldsymbol{y}, \xi) = \int_{\mathbb{R}^d} p(\boldsymbol{s}, \xi) \overline{\varphi_1(\boldsymbol{y} - \boldsymbol{s})} \varphi_2(\boldsymbol{x} - \boldsymbol{s}) \,\mathrm{d}\boldsymbol{s}.$$

This implies (e.g., see Martinez, 2001, Theorem 2.7.1, which uses the same convention as here) that $\mathscr{F}_{\varphi_2}^* p \mathscr{F}_{\varphi_1} = \operatorname{op}[b_{1/2}]$, where

$$\begin{aligned}b_{1/2}(\boldsymbol{x}, \xi) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\xi'-\xi)\cdot\boldsymbol{t}} b(\boldsymbol{x} + \tfrac{1}{2}\boldsymbol{t}, \boldsymbol{x} - \tfrac{1}{2}\boldsymbol{t}, \xi') \,\mathrm{d}\xi'\,\mathrm{d}\boldsymbol{t} \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}(\xi'-\xi)\cdot\boldsymbol{t}} p(\boldsymbol{s}, \xi') \overline{\varphi_1(\boldsymbol{x} - \tfrac{1}{2}\boldsymbol{t} - \boldsymbol{s})} \varphi_2(\boldsymbol{x} + \tfrac{1}{2}\boldsymbol{t} - \boldsymbol{s}) \,\mathrm{d}\boldsymbol{s}\,\mathrm{d}\xi'\,\mathrm{d}\boldsymbol{t} \\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} p(\boldsymbol{s}, \xi') \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{x} - \boldsymbol{s}, \xi - \xi') \,\mathrm{d}\boldsymbol{s}\,\mathrm{d}\xi' = \mathscr{W}_{\varphi_2,\varphi_1} * p(\boldsymbol{x}, \xi).\end{aligned}$$

□

We will need the following basic properties of $\mathscr{W}_{\varphi_2,\varphi_1}$:

1. If $\varphi_1, \varphi_2 \in \mathscr{S}(\mathbb{R}^{2d})$ then $\mathscr{W}_{\varphi_2,\varphi_1} \in \mathscr{S}(\mathbb{R}^{2d})$.

2. For all $\boldsymbol{x} \in \mathbb{R}^d$ we have $\int_{\mathbb{R}^d} \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{x},\xi)\,\mathrm{d}\xi = \varphi_2(\boldsymbol{x})\overline{\varphi_1(\boldsymbol{x})}$.

3. We have $\mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{z}) = \overline{\mathscr{W}_{\varphi_1,\varphi_2}(\boldsymbol{z})}$. (Note the transposed positions of φ_1, φ_2.)

These properties follow easily from the definition of $\mathscr{W}_{\varphi_2,\varphi_1}$ (see for example Folland, 1989, §1.8).

Proof of Lemma 5.4.1. This is an immediate consequence of the above properties of $\mathscr{W}_{\varphi_2,\varphi_1}$. $\square$

We will need a fourth property of the Wigner transform in order to prove Lemma 5.4.2: its relationship with the fractional Fourier transform, which is defined as follows.

Definition 5.4.5. For any $t \in \mathbb{R}$, we define the fractional Fourier transform $\mathscr{F}^t : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ to be the operator with Schwartz kernel

$$k(x,y) := \sum_{n=0}^{\infty} \mathrm{e}^{-\mathrm{i}tn\pi/2} \psi_n(x)\psi_n(y),$$

where ψ_n are the appropriately scaled Hermite functions (in this document, following the convention in Lemma 5.5.1).

For more information about the fractional Fourier transform, including the definition of the Hermite functions, the reader is referred to the review article by Ozaktas, Kutay and Mendlovic (1999) or the book by Ozaktas, Kutay and Zalevsky (2001, Chapter 4) on the subject. Of particular note is that when $t = 1$ this is the usual Fourier transform. For other $t \in \mathbb{R}$ the definition is similar to functions of self-adjoint operators in terms of the spectral theorem, but because the Fourier transform is unitary a branch of the power function must be chosen; with the fractional Fourier transform, a different branch is chosen for every eigenvalue (eventually cycling if t is rational). It satisfies the key additivity property that $\mathscr{F}^{t_1}\mathscr{F}^{t_2} = \mathscr{F}^{t_1+t_2}$, with $\mathscr{F}^4 = \mathscr{F}^0 = \mathrm{Id}_{L^2(\mathbb{R})}$; we may therefore index by direction $\boldsymbol{\omega} \in \mathbb{S}^1$, so that $\mathscr{F}^{(1,0)} = \mathrm{Id}_{L^2(\mathbb{R})}$ and $\mathscr{F}^{(0,1)} = \mathscr{F}$.

The fourth property of $\mathscr{W}_{\varphi_2,\varphi_1}$ is as follows.

4. ($d = 1$.) For each $\boldsymbol{\omega} \in \mathbb{S}^1$, let $\sigma_{\boldsymbol{\omega}} : \mathbb{R}^2 \to \mathbb{R}^2$ be the rotation that maps $(1,0) \mapsto \boldsymbol{\omega}$; then for all $\boldsymbol{z} \in \mathbb{R}^2$ we have $\mathscr{W}_{\varphi_2,\varphi_1}(\sigma_{\boldsymbol{\omega}}\boldsymbol{z}) = \mathscr{W}_{\mathscr{F}^{\boldsymbol{\omega}}\varphi_2,\mathscr{F}^{\boldsymbol{\omega}}\varphi_1}(\boldsymbol{z})$.

In others words, the fractional Fourier transform is the metaplectic operator corresponding to rotation. For example, in Folland (1989) see Proposition (1.94)(c) for the $\boldsymbol{\omega} = (1,0)$ case (the usual Fourier transform) and Chapter 4 for discussion of metaplectic operators (especially Proposition (4.28) for the relationship to the Wigner transform), in Ozaktas, Kutay and Mendlovic (1999) see §7, and in Ozaktas, Kutay and Zalevsky (2001) see §4.6.1.

In higher dimensions a similar result holds component-wise (as also discussed in those references). We define the component-wise fractional Fourier transform in the obvious way; explicitly, for $j \in \{1,\dots,d\}$ it is

$$\mathscr{F}_j^{\boldsymbol{\omega}} u(\boldsymbol{x}) := \mathscr{F}^{\boldsymbol{\omega}}(x_j \mapsto u(\boldsymbol{x})).$$

The corresponding property of $\mathscr{W}_{\varphi_2,\varphi_1}$ is as follows.

4. (General d.) Let $\boldsymbol{\nu} \in \mathbb{S}^1$ and $j \in \{1,\dots,d\}$. Let $\sigma : \mathbb{R}^2 \to \mathbb{R}^2$ be the rotation that maps $(1,0) \mapsto \boldsymbol{\nu}$, and let $\tau : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be the rotation such that for each $i \neq j$

$$\big(((\tau(\boldsymbol{z}))_1)_j, ((\tau(\boldsymbol{z}))_2)_j\big) = \sigma\big((\boldsymbol{z}_1)_j, (\boldsymbol{z}_2)_j\big), \qquad \big(((\tau(\boldsymbol{z}))_1)_i, ((\tau(\boldsymbol{z}))_2)_i\big) = \big((\boldsymbol{z}_1)_i, (\boldsymbol{z}_2)_i\big);$$

in other words, τ rotates the j^{th} component in the same manner as σ, and leaves other components unchanged. Then for all $\boldsymbol{z} \in \mathbb{R}^2$ we have $\mathscr{W}_{\varphi_2,\varphi_1}(\tau \boldsymbol{z}) = \mathscr{W}_{\mathscr{F}_j^{\boldsymbol{\nu}}\varphi_2, \mathscr{F}_j^{\boldsymbol{\nu}}\varphi_1}(\boldsymbol{z})$.

We are now ready to prove Lemma 5.4.2.

Proof of Lemma 5.4.2. One-dimensional case. Applying property 4 of $\mathscr{W}_{\varphi_2,\varphi_1}$ and then changing variables $\boldsymbol{z}' = \sigma_{\boldsymbol{\omega}}(\boldsymbol{v})$ we obtain

$$\begin{aligned}\int_{\{\boldsymbol{z}' \in \mathbb{R}^2 : \boldsymbol{z}' \cdot \boldsymbol{\omega} = \lambda\}} \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{z}')\mu_1(\mathrm{d}\boldsymbol{z}') &= \int_{\{\boldsymbol{z}' \in \mathbb{R}^2 : \boldsymbol{z}' \cdot \boldsymbol{\omega} = \lambda\}} \mathscr{W}_{\mathscr{F}^{\boldsymbol{\omega}}\varphi_2, \mathscr{F}^{\boldsymbol{\omega}}\varphi_1}(\sigma_{\boldsymbol{\omega}}^{-1}(\boldsymbol{z}'))\mu_1(\mathrm{d}\boldsymbol{z}') \\ &= \int_{\{\boldsymbol{v} \in \mathbb{R}^2 : \sigma_{\boldsymbol{\omega}}(\boldsymbol{v}) \cdot \boldsymbol{\omega} = \lambda\}} \mathscr{W}_{\mathscr{F}^{\boldsymbol{\omega}}\varphi_2, \mathscr{F}^{\boldsymbol{\omega}}\varphi_1}(\boldsymbol{v})\mu_1(\mathrm{d}\boldsymbol{v}).\end{aligned}$$

But $\boldsymbol{\omega} = \sigma_{\boldsymbol{\omega}}(1,0)$, so

$$\sigma_{\boldsymbol{\omega}}(\boldsymbol{v}) \cdot \boldsymbol{\omega} = \sigma_{\boldsymbol{\omega}}(\boldsymbol{v}) \cdot \sigma_{\boldsymbol{\omega}}(1,0) = \boldsymbol{v} \cdot (1,0) = v_1,$$

so this is the integral over all v_2 such that $v_1 = \lambda$. Applying property 2 of $\mathscr{W}_{\varphi_2,\varphi_1}$ gives

$$\int_{\{\boldsymbol{z}' \in \mathbb{R}^2 : \boldsymbol{z}' \cdot \boldsymbol{\omega} = \lambda\}} \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{z}')\mu_1(\mathrm{d}\boldsymbol{z}') = \mathscr{F}^{\boldsymbol{\omega}}\varphi_2(\lambda)\overline{\mathscr{F}^{\boldsymbol{\omega}}\varphi_1(\lambda)}.$$

(This is sometimes call the Radon–Wigner transform, since it is the Radon transform of the Wigner distribution.) But $Q_{\boldsymbol{\omega}}$ is the antiderivative of this expression, so when $\varphi_1 = \varphi_2$ it is non-decreasing.

General dimension. Let $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$. For each $j \in \{1,\dots,d\}$ there are rotations

$$\sigma_j : \mathbb{R}^2 \to \mathbb{R}^2,\ \sigma_j^{-1}\big((\boldsymbol{\omega}_1)_j, (\boldsymbol{\omega}_2)_j\big) = (W_j, 0),$$

where $W_j := \big|\big((\boldsymbol{\omega}_1)_j, (\boldsymbol{\omega}_2)_j\big)\big| = \sqrt{(\boldsymbol{\omega}_1)_j^2 + (\boldsymbol{\omega}_2)_j^2}$. If $\big((\boldsymbol{\omega}_1)_j, (\boldsymbol{\omega}_2)_j\big) \neq (0,0)$ ($\Leftrightarrow W_j \neq 0$) then this rotation is uniquely defined; otherwise set it to the identity function (i.e. null rotation). Denote

$$\tilde{\boldsymbol{\omega}} := (W_1, \dots, W_d) \in \mathbb{S}^{d-1} \quad \text{and} \quad T_{\boldsymbol{\omega}} := \mathscr{F}_d^{\sigma_d(1,0)} \dots \mathscr{F}_1^{\sigma_1(1,0)}.$$

Then, applying property 4 as in the one-dimensional case,

$$\int_{\{\boldsymbol{z}' \in \mathbb{R}^{2d} : \boldsymbol{z}' \cdot \boldsymbol{\omega} = \lambda\}} \mathscr{W}_{\varphi_2,\varphi_1}(\boldsymbol{z}')\mu_{2d-1}(\mathrm{d}\boldsymbol{z}') = \int_{\{\boldsymbol{x} \in \mathbb{R}^d : \boldsymbol{x} \cdot \tilde{\boldsymbol{\omega}} = \lambda\}} T_{\boldsymbol{\omega}}\varphi_2(\boldsymbol{x})\overline{T_{\boldsymbol{\omega}}\varphi_2(\boldsymbol{x})}\mu_{d-1}(\mathrm{d}\boldsymbol{x}).$$

Thus
$$Q_{\boldsymbol{\omega}}(\lambda) = \int_{-\infty}^{\lambda} \int_{\{\boldsymbol{x}\in\mathbb{R}^d : \boldsymbol{x}\cdot\tilde{\boldsymbol{\omega}}=\eta\}} T_{\boldsymbol{\omega}}\varphi_2(\boldsymbol{x})\overline{T_{\boldsymbol{\omega}}\varphi_1(\boldsymbol{x})}\mu_{d-1}(\mathrm{d}\boldsymbol{x})\,\mathrm{d}\eta,$$
so when $\varphi_1 = \varphi_2$ this is a non-decreasing function. □

The proof of Lemma 5.4.3 requires a property about generalised anti-Wick operators other than their connection to the Weyl quantisation: that if $a \geqslant 0$ then the operator $\mathscr{A}_\varphi[a]$ is positive. This is a standard fact, and indeed one of the most well-known uses of anti-Wick operators is to prove Gårding's inequality using it (Tulovsky and Shubin, 1973, §2). It is easily verified directly, by observing that
$$\langle \mathscr{A}_\varphi[a]u, u\rangle_{L^2(\mathbb{R}^d)} = \langle \mathscr{F}_\varphi^* a \mathscr{F}_\varphi u, u\rangle_{L^2(\mathbb{R}^d)} = \langle a\mathscr{F}_\varphi u, \mathscr{F}_\varphi u\rangle_{L^2(\mathbb{R}^{2d})} = \int_{\mathbb{R}^{2d}} a(\boldsymbol{z})|\mathscr{F}_\varphi u(\boldsymbol{z})|^2\,\mathrm{d}\boldsymbol{z} \geqslant 0.$$
(Here $\mathscr{F}_\varphi$ is again the short-time Fourier transform with window φ, rather than the fractional Fourier transform $\mathscr{F}^t$.)

Proof of Lemma 5.4.3. Let $\ell := \min\{0, c\}$ (where $a(\boldsymbol{z}) \geqslant c > -1$). Set $f(t) := \log(1+t)$, and let $\tilde{f} \in C^\infty(\mathbb{R})$ such that
$$\tilde{f}(t) = \log(1+t) \qquad \text{when } t \geqslant \ell.$$
The generalised anti-Wick symbol of $T_r[a\chi_\Omega] - \ell I$ is $(a\chi_\Omega)_r - \ell$, which is positive, so $f(T_r[a\chi_\Omega]) = \tilde{f}(T_r[a\chi_\Omega])$. We may therefore apply Theorem 5.2.6 or Theorem 5.2.8 (with $\tilde{f}$) giving
$$\operatorname{tr} f(T_r[a\chi_\Omega]) = r^{2d}A_0(a, \Omega, \tilde{f}) + r^{2d-1}A_1(a, \Omega, \tilde{f}; W) + O(r^{2d-2})$$
as $r \to \infty$. But A_0 only depends on $\tilde{f}(t)$ for t in the image of a. As shown in Lemma 5.4.2, the function $Q_{\boldsymbol{\omega}}$ is increasing; this implies that $0 \leqslant Q_{\boldsymbol{\omega}}(\lambda) \leqslant 1$ for all $\lambda \in [0,1]$ and $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$, so A_1 also only depends on $\tilde{f}(t)$ for t in the image of a. Thus
$$A_0(a, \Omega, \tilde{f}) = A_0(a, \Omega, f), \qquad A_1(a, \Omega, \tilde{f}; W) = A_1(a, \Omega, f; W).$$ □

5.5 Spherically symmetric convolution factor

In this section we note two special cases of generalised anti-Wick operators of particular interest. Both of these have spherically symmetric convolution factors; that is, $W(\boldsymbol{u}) = W(\boldsymbol{v})$ whenever $|\boldsymbol{u}| = |\boldsymbol{v}|$. Having stated the two special cases we will make some minor observations that apply to any $T_r[p]$ with spherically-symmetric W.

The most important special case of the operator $T_r[p]$ is the class of anti-Wick operators (as opposed to generalised anti-Wick operators) as originally studied (see §1.4). Here the window is the appropriately-scaled Gaussian (L^2 normalised), and then W is also a Gaussian (L^1 normalised). The precise meaning of "appropriately-scaled" with the conventions used in this document is given Lemma 5.5.1 at the end of this section.

Another class of windows for which $\mathscr{W}_\varphi$ is spherically symmetric is the set of (appropriately scaled) Hermite functions in one dimension. See for example Folland (1989, Theorem (1.105)), and see Pushnitski, Raikov and Villegas-Blas (2013, §2.3) for an example of their use in generalised anti-Wick operators.

When W is spherically symmetric, the function $Q_{\boldsymbol{\omega}}(\lambda)$ has no dependence on the direction $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$ and we write simply $Q(\lambda)$. Then:

- The asymptotic term A_1 can be written in the alternative form $\tilde{A}_1$ (see Lemma 5.8.3).
- For $p \in \mathscr{S}(\mathbb{R}^{2d})$, the operator $T_r[p]$ is r^2-admissible when a is smooth (see Lemma 5.7.1 and comments after it).
- If, in addition, the smooth part of the symbol a equals a constant c, then the integrand in the asymptotic term A_1 has no dependence on $\boldsymbol{u} \in \partial\Omega$, so it is proportional to the measure of $\partial\Omega$. It is also clear that when a is constant the term A_0 is proportional to the measure of Ω (even if W is not spherically symmetric). Explicitly,

$$A_0(a,\Omega,f) = \frac{1}{(2\pi)^d}\mu_{2d}(\Omega)f(c),$$
$$A_1(a,\Omega,f;W) = \frac{1}{(2\pi)^d}\mu_{2d-1}(\partial\Omega)\int_{\mathbb{R}}\Big(f(cQ(\lambda)) - Q(\lambda)f(c)\Big)\mathrm{d}\lambda.$$

  This includes $f = \chi_{[\delta,\infty)}$ as in Corollary 5.3.1. If, in addition, $Q(\lambda)$ is an increasing function (as discussed in Remark 5.3.2) then it immediately follows that the asymptotic terms take the particularly simple form

$$A_0(a,\Omega,\chi_{[\delta,\infty)}) = \frac{1}{(2\pi)^d}\mu_{2d}(\Omega),$$
$$A_1(a,\Omega,\chi_{[\delta,\infty)};W) = -\frac{1}{(2\pi)^d}\mu_{2d-1}(\partial\Omega)Q^{-1}(\delta).$$

Finally, as promised at the start of this section, we give the precise form of the window function φ and Wigner transform $\mathscr{W}_\varphi$ for anti-Wick operators.

Lemma 5.5.1. *We have*

$$\varphi(\boldsymbol{x}) := \frac{1}{\pi^{d/4}}\mathrm{e}^{-|\boldsymbol{x}|^2/2} \quad \Longrightarrow \quad \mathscr{W}_\varphi(\boldsymbol{z}) = \frac{1}{\pi^d}\mathrm{e}^{-|\boldsymbol{z}|^2},\ Q(\lambda) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\lambda}\mathrm{e}^{-t^2}\,\mathrm{d}t.$$

Furthermore, with this choice of φ we have $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$ and $\|\mathscr{W}_\varphi\|_{L^1(\mathbb{R}^{2d})} = 1$.

Proof. Fourier transform of Gaussian. We will first need to recall the standard integral used in the Fourier transform of the Gaussian function (which gives the integral of the Gaussian by substituting $\boldsymbol{\eta}=\mathbf{0}$). The formula (Folland, 1989, Appendix A), for each $\beta>0$, is

$$\int_{\mathbb{R}^d} \mathrm{e}^{-\pi\beta|\boldsymbol{x}|^2-2\pi\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{\eta}}\,\mathrm{d}\boldsymbol{x}=\frac{1}{\beta^{d/2}}\mathrm{e}^{-\pi|\boldsymbol{\eta}|^2/\beta}.$$

We will need to rescale this so that it is easier to use with the convention of the Fourier transform used here. Writing the scaling constant as $(2\pi)^2/\kappa=\pi\beta$ (so that $\beta=4\pi/\kappa$) we obtain

$$\int_{\mathbb{R}^d} \mathrm{e}^{-(2\pi)^2|\boldsymbol{x}|^2/\kappa-2\pi\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{\eta}}\,\mathrm{d}\boldsymbol{x}=\left(\frac{\kappa}{4\pi}\right)^{d/2}\mathrm{e}^{-\kappa|\boldsymbol{\eta}|^2/4}.$$

Now changing variables $\boldsymbol{t}:=2\pi\boldsymbol{x}$ we find that

$$\int_{\mathbb{R}^d} \mathrm{e}^{-|\boldsymbol{t}|^2/\kappa}\mathrm{e}^{-\mathrm{i}\boldsymbol{t}\cdot\boldsymbol{\eta}}\,\mathrm{d}\boldsymbol{t}=(2\pi)^d\left(\frac{\kappa}{4\pi}\right)^{d/2}\mathrm{e}^{-|\boldsymbol{\eta}|^2/4\kappa}=(\kappa\pi)^{d/2}\mathrm{e}^{-|\boldsymbol{\eta}|^2/4\kappa}.$$

Expression for $\mathscr{W}_\varphi$. First note that the exponent of $\varphi(\boldsymbol{z}_1+\frac{1}{2}\boldsymbol{t})\overline{\varphi(\boldsymbol{z}_1-\frac{1}{2}\boldsymbol{t})}$ is

$$-\tfrac{1}{2}\left(\left|\boldsymbol{z}_1+\tfrac{1}{2}\boldsymbol{t}\right|^2+\left|\boldsymbol{z}_1-\tfrac{1}{2}\boldsymbol{t}\right|^2\right)=-\tfrac{1}{2}\left(|\boldsymbol{z}_1|^2+\boldsymbol{z}_1\cdot\boldsymbol{t}+\tfrac{1}{4}|\boldsymbol{t}|^2+|\boldsymbol{z}_1|^2-\boldsymbol{z}_1\cdot\boldsymbol{t}+\tfrac{1}{4}|\boldsymbol{t}|^2\right)=-\left(|\boldsymbol{z}_1|^2+\tfrac{1}{4}|\boldsymbol{t}|^2\right).$$

Thus (using $\kappa=4$)

$$\begin{aligned}\mathscr{W}_\varphi(\boldsymbol{z})&=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\mathrm{e}^{-\mathrm{i}\boldsymbol{t}\cdot\boldsymbol{z}_2}\varphi(\boldsymbol{z}_1+\tfrac{1}{2}\boldsymbol{t})\overline{\varphi(\boldsymbol{z}_1-\tfrac{1}{2}\boldsymbol{t})}\,\mathrm{d}\boldsymbol{t}\\&=\frac{1}{(2\pi)^d}\frac{1}{\pi^{d/2}}\mathrm{e}^{-|\boldsymbol{z}_1|^2}\int_{\mathbb{R}^d}\mathrm{e}^{-\mathrm{i}\boldsymbol{t}\cdot\boldsymbol{z}_2}\mathrm{e}^{-|\boldsymbol{t}|^2/4}\,\mathrm{d}\boldsymbol{t}\\&=\frac{1}{(2\pi)^d}\frac{1}{\pi^{d/2}}\mathrm{e}^{-|\boldsymbol{z}_1|^2}(4\pi)^{d/2}\mathrm{e}^{-|\boldsymbol{z}_2|^2}=\frac{1}{\pi^d}\mathrm{e}^{-|\boldsymbol{z}|^2}.\end{aligned}$$

Norms of φ and $\mathscr{W}_\varphi$. We have (using $\kappa=1$)

$$\|\varphi\|^2_{L^2(\mathbb{R}^d)}=\frac{1}{\pi^{d/2}}\int_{\mathbb{R}^d}\mathrm{e}^{-|\boldsymbol{x}|^2}\,\mathrm{d}\boldsymbol{x}=1,$$

and (using $\kappa=1$ again, in $2d$ dimensions)

$$\|\mathscr{W}_\varphi\|_{L^1(\mathbb{R}^{2d})}=\frac{1}{\pi^d}\int_{\mathbb{R}^{2d}}\mathrm{e}^{-|\boldsymbol{z}|^2}\,\mathrm{d}\boldsymbol{z}=1.$$

Expression for Q. Because $\mathscr{W}_\varphi$ is spherically symmetric, it is immediate that $Q_{\boldsymbol{\omega}}$ does not depend on the direction $\boldsymbol{\omega}\in\mathbb{S}^{2d-1}$. Evaluating with $\boldsymbol{\omega}=\mathbf{e}_1$, we find

$$Q(\lambda)=\left(\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\lambda}\mathrm{e}^{-x_1^2}\,\mathrm{d}x_1\right)\left(\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-x_2^2}\,\mathrm{d}x_2\right)\cdots\left(\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-x_{2d}^2}\,\mathrm{d}x_{2d}\right).$$

Every factor except for the first equals 1, so we arrive at the stated expression. $\square$

5.6 Szegő theorem with cusps

The Szegő theorem stated in §5.2 includes the requirement that Ω is a Lipschitz domain; this excludes the possibility of cusps in the boundary. In this section we state a result that shows that the Szegő expansion is different when there is a cusp: it has the same leading term and boundary term, but there is an extra contribution that is larger than the $O(r^{2d-2})$ remainder of the main theorem. At the end of this section there is an outline of the proof, and the full proof is in §6.6.

The main purpose of this cusp result is to show that some of the conditions in the main result in §5.2 really are necessary; it does not hold in the same form for an arbitrary domain $\Omega \subseteq \mathbb{R}^{2d}$. For this reason the result in this section is proved under some restrictive assumptions that simplify the proof but still make this point. Some of them, in the author's opinion, probably do not affect the Szegő expansion; the assumption that $\omega''(0) = 0$, which excludes $\omega(x) = x^2$, is particularly artificial. The condition that W is compact, which excludes the possibility that $T_r[\chi_\Omega a]$ is a generalised anti-Wick operator, is also unlikely to be important. In contrast, the assumption that the function of the operator is $f(t) = t^2$ is much more severe; it is possible that Szegő expansion takes a special form for this particular f. However, this makes the proof straightforward because the most difficult part, finding the trace of $f(T_r[a\chi_\Omega])$ as an explicit integral, is trivial with this choice of f.

To state the cusp result we make use of another asymptotic notation: we write

$$f(x) = g(x) + \Theta(r(x)) \quad \Longleftrightarrow \quad C_1|r(x)| \leqslant |f(x) - g(x)| \leqslant C_2|r(x)|,$$

where $C_1, C_2 > 0$ and the inequalities hold for all sufficiently large x. This relationship is sometimes expressed with the alternative notation $f(x) - g(x) \asymp r(x)$.

Theorem 5.6.1. *Let $d = 1$. Let $f(t) = t^2$. Let the following conditions all be satisfied:*

- *Let $W \in \mathscr{S}(\mathbb{R}^2)$ satisfy $W(\mathbf{0}) > 0$ and $\int_{\mathbb{R}^2} W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, and let it be compactly supported.*
- *Let $a \in C^2(\mathbb{R}^2)$ be real valued and have no dependence on the second variable (i.e. $a(x, y) = a(x, 0)$ for all $x, y \in \mathbb{R}$) and satisfy*

$$a(x, y) = \begin{cases} 1 & \text{when } x \leqslant 2, \\ 0 & \text{when } x \geqslant 3. \end{cases}$$

- *Let $\Omega \subseteq \mathbb{R}^2$ be a region with a cusp of the following form. Let $\omega \in C^2(\mathbb{R})$ satisfy*

$$\omega(x) = 0 \quad \text{when } x \leqslant 0,$$
$$\omega(x) > 0 \quad \text{when } 0 < x < 1,$$
$$\omega(x) = 1 \quad \text{when } x \geqslant 1,$$

which implies that $\omega(0) = \omega'(0) = \omega''(0) = 0$. Furthermore, let ω be a convex function on $[0, k)$ for some $k > 0$, which implies that ω is strictly increasing and invertible on $[0, k)$.

Denote

$$\Omega_1 := \{(x,y)\in\mathbb{R}^2 : x\geqslant 0,\ y\leqslant\omega(x)\},$$
$$\Omega_2 := \{(x,y)\in\mathbb{R}^2 : x\geqslant 0,\ y\geqslant 0\},$$

and define $\Omega := \Omega_1\cap\Omega_2$.

Then

$$\operatorname{tr} f(T_r[\chi_\Omega a]) = r^2 A_0(a,\Omega,f) + r A_1(a,\Omega,f;W) + \Theta\left(r\,\omega^{-1}\left(\frac{1}{r}\right)\right)$$

as $r\to\infty$.

For example, for $n\geqslant 3$, for all sufficiently small x,

$$\omega(x) = x^n \quad\Longrightarrow\quad \text{remainder} = \Theta\left(\frac{r}{\sqrt[n]{r}}\right),$$
$$\omega(x) = \exp\left(-\frac{1}{x}\right) \quad\Longrightarrow\quad \text{remainder} = \Theta\left(\frac{r}{\log r}\right).$$

Here is a brief outline of the proof of Theorem 5.6.1; the complete proof is in §6.6. It follows the same general outline as the proof of the main result, which is discussed at the start of Chapter 6. As noted earlier in this section, the composition part of the proof will turn out to be trivial for this choice of f. The next part involves simplifying an integral that is approximately equal to A_1. Its integrand is non-zero on a strip around $\partial\Omega$, while A_1 may be considered as a sum of integrals whose integrands are non-zero on strips around $\partial\Omega_1$ and $\partial\Omega_2$. Bounding W above and below by indicator functions, their difference is therefore related to the overlap of the two strips, which is

$$\begin{aligned} R &= r c\int_0^\infty\int_{-\infty}^\infty \chi_{[-s,\infty)}(y - r\,\omega(x))\,\chi_{[-s,\infty)}(-y)\,\mathrm{d}y\,\mathrm{d}x \\ &= \Theta\left(r\int_0^\infty \chi_{(-\infty,2s]}(r\,\omega(x))\,\mathrm{d}x\right). \end{aligned}$$

(In fact, the strip width s and constant factor c differ for the upper and lower bounds of the remainder.) Up until this point (the end of step 4 in the proof), no use is made of the assumption that ω is convex near to 0; for example, it applies when $\omega(x) = x^3(2+\sin(1/x))$. The end of the proof (steps 5 and 6) uses the convexity assumption with this bound to show that $R = \Theta(r\,\omega^{-1}(1/r))$.

5.7 Idea of proof

In §2.4 we discussed how, in approximating the composition of pseudodifferential operators by an asymptotic series, the remainder is usually bounded using ideas encapsulated in Lemma 2.4.2. As promised then, we now discuss how this does not work for the main result of this thesis, where the operator is $T_r[p]$ with discontinuous p, and give an idea of how the more delicate bound proved in §2.3 can be used instead.

First, for contrast, we consider $T_r[p]$ where p is smooth. In this case the ideas of §2.3 do apply, as the lemma below shows.

Lemma 5.7.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ with integral equal to 1 and $p \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$. Then for each $n \in \mathbb{N}$ we have*

$$T_r[p] = \sum_{j=0}^{n} \frac{1}{r^j} \operatorname{op}^{\mathrm{W}}_{1/r^2}[a_j(\boldsymbol{z})] + \frac{1}{r^{n+1}} \operatorname{op}^{\mathrm{W}}_{1/r^2}[R_{n+1}(\boldsymbol{z}; r)],$$

where

$$a_j(\boldsymbol{z}) = \frac{1}{j!} \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}')\big((-\boldsymbol{z}' \cdot \nabla)^j p\big)(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z}',$$

$$R_{n+1}(\boldsymbol{z}; r) = \frac{1}{n!} \int_0^1 \int_{\mathbb{R}^{2d}} (1-t)^n W(\boldsymbol{z}')\big((-\boldsymbol{z}' \cdot \nabla)^{n+1} p\big)\Big(\boldsymbol{z} - t\frac{\boldsymbol{z}'}{r}\Big)\, \mathrm{d}\boldsymbol{z}'\, \mathrm{d}t.$$

In particular, $a_0 = p$.

Furthermore, let m be an order function (see Definition 2.4.6) and $p \in S(m)$ (see Definition 2.4.8). Then $a_j \in S(m)$ and $R_{n+1}(\boldsymbol{z}; r) \in S(m)$.

Remark 5.7.2. At first glance, this might appear to contradict Lemma 5.1.3, which says that the trace of $T_r[p]$ is precisely equal to a multiple of r^{2d}. But, although the a_j are not necessarily zero, their integrals are zero for $j > 0$. This can be seen by noting that the integral of each a_j is a sum of terms that each include a factor of the form

$$\int_{\mathbb{R}^{2d}} \partial^{\boldsymbol{k}} p(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z},$$

with $|\boldsymbol{k}| = j$. First evaluating the $\mathrm{d}z_m$ integral, where m is chosen so that $k_m \neq 0$, by the fundamental theorem of calculus we find that this integral equals zero.

Proof. Series expansion. We have

$$W * p_r(\boldsymbol{z}) = \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}') p\Big(\frac{\boldsymbol{z}-\boldsymbol{z}'}{r}\Big)\, \mathrm{d}\boldsymbol{z}' = q\Big(\frac{\boldsymbol{z}}{r}; r\Big), \quad \text{where } q(\boldsymbol{z}; r) := \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}') p\Big(\boldsymbol{z} - \frac{\boldsymbol{z}'}{r}\Big)\, \mathrm{d}\boldsymbol{z}'.$$

Thus

$$T_r[p] = \operatorname{op}[W * p_r] = \operatorname{op}\Big[q\Big(\frac{\boldsymbol{z}}{r}; r\Big)\Big] = \operatorname{op}^{\mathrm{W}}_{1/r^2}[q(\boldsymbol{z}; r)].$$

Taylor's theorem says that

$$p(\boldsymbol{z} + \boldsymbol{x}) = \sum_{j=0}^{n} \frac{1}{j!}\big((\boldsymbol{x} \cdot \nabla)^j p\big)(\boldsymbol{z}) + \frac{1}{n!} \int_0^1 (1-t)^n \big((\boldsymbol{x} \cdot \nabla)^{n+1} p\big)(\boldsymbol{z} + t\boldsymbol{x})\, \mathrm{d}t,$$

and putting $\boldsymbol{x} = -\boldsymbol{z}'/r$ and substituting into q gives the stated series and remainder.

Bounds by order function. The multinomial theorem says that

$$(-\boldsymbol{z}' \cdot \nabla)^j = (-1)^j \sum_{|\boldsymbol{k}|=j} \binom{j}{\boldsymbol{k}} (\boldsymbol{z}')^{\boldsymbol{k}} \partial^{\boldsymbol{k}},$$

so

$$
\begin{aligned}
|\partial^{\boldsymbol{m}} a_j(\boldsymbol{z})| &\leqslant \frac{1}{j!} \sum_{|\boldsymbol{k}|=j} \binom{j}{\boldsymbol{k}} \int_{\mathbb{R}^{2d}} |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}') \partial^{\boldsymbol{k}+\boldsymbol{m}} p(\boldsymbol{z})| \, \mathrm{d}\boldsymbol{z}' \\
&\leqslant m(\boldsymbol{z}) \frac{1}{j!} \sum_{|\boldsymbol{k}|=j} \binom{j}{\boldsymbol{k}} \int_{\mathbb{R}^{2d}} C_{\boldsymbol{k}+\boldsymbol{m}} |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}')| \, \mathrm{d}\boldsymbol{z}'.
\end{aligned}
$$

For the remainder bound, first observe that

$$
\begin{aligned}
|\partial^{\boldsymbol{m}} R_{n+1}(\boldsymbol{z}; r)| &\leqslant \frac{1}{n!} \sum_{|\boldsymbol{k}|=n+1} \binom{n+1}{\boldsymbol{k}} \int_0^1 \int_{\mathbb{R}^{2d}} \left| (1-t)^n (\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}') \partial^{\boldsymbol{k}+\boldsymbol{m}} p\Big(\boldsymbol{z} - t\frac{\boldsymbol{z}'}{r}\Big) \right| \mathrm{d}\boldsymbol{z}' \, \mathrm{d}t \\
&\leqslant \frac{1}{n!} \sum_{|\boldsymbol{k}|=n+1} \binom{n+1}{\boldsymbol{k}} \int_0^1 \int_{\mathbb{R}^{2d}} (1-t)^n C_{\boldsymbol{k}+\boldsymbol{m}} |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}')| m\Big(\boldsymbol{z} - t\frac{\boldsymbol{z}'}{r}\Big) \mathrm{d}\boldsymbol{z}' \, \mathrm{d}t.
\end{aligned}
$$

But m is an order function, so for $r \geqslant 1$ we have

$$
\begin{aligned}
|\partial^{\boldsymbol{m}} R_{n+1}(\boldsymbol{z}; r)| &\leqslant \frac{1}{n!} C_0 m(\boldsymbol{z}) \sum_{|\boldsymbol{k}|=n+1} \binom{n+1}{\boldsymbol{k}} \int_0^1 \int_{\mathbb{R}^{2d}} (1-t)^n C_{\boldsymbol{k}+\boldsymbol{m}} \Big\langle t\frac{\boldsymbol{z}'}{r} \Big\rangle^N |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}')| \, \mathrm{d}\boldsymbol{z}' \, \mathrm{d}t \\
&\leqslant \frac{1}{n!} C_0 m(\boldsymbol{z}) \sum_{|\boldsymbol{k}|=n+1} \binom{n+1}{\boldsymbol{k}} \int_0^1 \int_{\mathbb{R}^{2d}} (1-t)^n C_{\boldsymbol{k}+\boldsymbol{m}} \langle \boldsymbol{z}' \rangle^N |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}')| \, \mathrm{d}\boldsymbol{z}' \, \mathrm{d}t \\
&= \frac{1}{(n+1)!} C_0 m(\boldsymbol{z}) \sum_{|\boldsymbol{k}|=n+1} \binom{n+1}{\boldsymbol{k}} \int_{\mathbb{R}^{2d}} C_{\boldsymbol{k}+\boldsymbol{m}} \langle \boldsymbol{z}' \rangle^N |(\boldsymbol{z}')^{\boldsymbol{k}} W(\boldsymbol{z}')| \, \mathrm{d}\boldsymbol{z}'. \qquad \square
\end{aligned}
$$

In the language of semiclassical analysis, the above lemma shows that $T_r[p]$ is r^2-admissible. In fact it is not quite in the traditional asymptotic form because the terms of an r^2-admissible operator should only have coefficients with even powers of r; however, the use of more general decreasing powers of r is a minor change that some authors allow (for example, Dimassi and Sjöstrand, 1999, comments before Proposition 7.6), and when W is spherically symmetric (as in §5.5) the odd-powered terms are zero so $T_r[p]$ really is r^2-admissible in the traditional sense.

The fact that $W * p_r$ is r^2-admissible for smooth p allows us to use the well-developed theory of semiclassical analysis on $T_r[p]$. However, for comparison with the case of discontinuous p it is more enlightening to look at the problem of composition directly, as done in the next lemma. As with the theory for symbol classes and semiclassical asymptotics, the only fact about the remainder needed in the proof of this lemma is the rough bound in Lemma 2.4.2.

Lemma 5.7.3. *Let $W, p \in \mathscr{S}(\mathbb{R}^{2d})$. Then*

$$
\left\| \big(\mathrm{op}[W * p_r]\big)^2 - \mathrm{op}\big[(W * p_r)^2\big] \right\|_1 \lesssim r^{2d-2} \|\nabla p\|_{L^\infty(\mathbb{R}^{2d})} \|\nabla p\|_{L^1(\mathbb{R}^{2d})}.
$$

Proof. We will apply Lemma 2.4.2 with $n = 0$ and $S = T = 2d+1$ and substitute into Lemma 2.1.3. By Lemma 5.1.2 we have

$$
\partial_j (W * p_r)(\boldsymbol{z}) = W * \big(\partial_{z_j} p_r(\boldsymbol{z})\big) = \frac{1}{r} W * \Big(\partial_j p\Big(\frac{\boldsymbol{z}}{r}\Big)\Big),
$$

so

$$\int_{\mathbb{R}^{2d}} \frac{|\partial^{\boldsymbol{k}}\partial_j(W*p_r)(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})|}{\langle\boldsymbol{x}\rangle^{2d+1}}\,\mathrm{d}\boldsymbol{x} \leqslant \frac{1}{r} I \sup|(\partial^{\boldsymbol{k}}W)*(\partial_j p)(\boldsymbol{z})| \lesssim \frac{1}{r}\|\nabla p\|_{L^\infty(\mathbb{R}^{2d})},$$

$$\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{|\partial^{\boldsymbol{k}}\partial_j(W*p_r)(\boldsymbol{z}-\sqrt{t}\boldsymbol{x})|}{\langle\boldsymbol{x}\rangle^{2d+1}}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z} = \frac{r^{2d}}{r} I \int_{\mathbb{R}^{2d}} |(\partial^{\boldsymbol{k}}W)*(\partial_j p)(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} \lesssim r^{2d-1}\|\nabla p\|_{L^1(\mathbb{R}^{2d})},$$

where I is the integral of $1/\langle\boldsymbol{x}\rangle^{2d-1}$. This gives the stated bound. □

When p is not smooth, the Weyl symbol $W*p_r$ is still a smooth function, but the reasoning used in Lemma 5.7.1 to show that $W*p_r$ is r^2-admissible no longer applies. Indeed the first term is p so would be discontinuous, and the second term involves derivatives of p so could be understood as a distribution but is not a function let alone a smooth one. Intuitively, the problem could be understood as being that the symbol depends upon two different scales in the phase space variable $\boldsymbol{z}$: when $\boldsymbol{z}$ is far from the boundary of Ω, $(a\chi_\Omega)_r(\boldsymbol{z})$ varies asymptotically like $a_r(\boldsymbol{z})$, so changes in $\boldsymbol{z}$ proportional to r are important; when $\boldsymbol{z}$ is near to the boundary it varies like $W*\chi_{r\Omega}(\boldsymbol{z})$, so changes in $\boldsymbol{z}$ on a constant scale are important.

The proof of Lemma 5.7.3 fails for discontinuous p because we now have, roughly speaking

$$\partial_j\big(W*(\chi_{r\Omega}a_r)\big) = \text{``}W*(\delta_{r\partial\Omega}a_r)\text{''} + W*(\chi_{r\Omega}\partial_j a_r),$$

where the notation $\delta_{r\partial\Omega}$ is used here to mean something like a Dirac delta sheet along $r\partial\Omega$. For example, if Ω is a half space then $W*\delta_{r\partial\Omega}$ is a smooth ridge running along the appropriate plane. The width of such a ridge is determined by W, so is constant as r grows, and so the integral is proportional to r^{2d-1} rather than r^{2d}. Continuing in the analogous way to Lemma 5.7.3 we end up with a trace norm bound that includes the four terms

$$\begin{aligned} r^{2d-2}\|\nabla a\|_{L^\infty(\Omega)}\|\nabla a\|_{L^1(\Omega)}, &\quad r^{2d-2}\|\nabla a\|_{L^\infty(\Omega)}\|a\|_{L^1(\partial\Omega)}, \\ r^{2d-2}\|a\|_{L^1(\partial\Omega)}\|\nabla a\|_{L^\infty(\Omega)}, &\quad r^{2d-1}\|a\|_{L^\infty(\partial\Omega)}\|a\|_{L^1(\partial\Omega)}. \end{aligned}$$

The focus of the proof of the Szegő theorem is therefore in obtaining a better bound for the fourth term so that its asymptotic order is r^{2d-2} as required.

- The proof of the rough estimate Lemma 2.4.2 involved taking the sum of absolute values of the terms that make up R_{n+1}. By using the more precise trace norm estimate Lemma 2.3.9 we may take advantage of cancellation between these terms, which gives the result when the boundary is smooth. This is done in §6.1.

- To deal with corners, rather than obtaining a bound $\|\cdots\|_{L^\infty}\|\cdots\|_{L^1}$ by taking the supremum of one factor and integrating over the other, we use the decay (of constant width) in both factors when integrating, giving an overall integral size of r^{2d-2} rather than r^{2d-1}. This is done in §6.4.

5.8 Boundary term properties

This section contains some facts about the boundary term A_1 that are needed elsewhere.

We often need to deal with the integral of $Q_{\boldsymbol{\omega}} - \chi_{[0,\infty)}$, and the following lemma gives important information about this.

Lemma 5.8.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ and set $U := \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'$. Then for all $\boldsymbol{\omega} \in \mathbb{S}^{2d-1}$ we have*

$$\int_{\mathbb{R}} (Q_{\boldsymbol{\omega}}(\lambda) - U\chi_{[0,\infty)}(\lambda))\,\mathrm{d}\lambda = -\int_{\mathbb{R}^{2d}} \boldsymbol{\omega}\cdot\boldsymbol{z}' W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',$$
$$\int_{\mathbb{R}} |Q_{\boldsymbol{\omega}}(\lambda) - U\chi_{[0,\infty)}(\lambda)|\,\mathrm{d}\lambda \leqslant \int_{\mathbb{R}^{2d}} |\boldsymbol{\omega}\cdot\boldsymbol{z}' W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}',$$
$$\int_{\mathbb{R}} |\lambda|\,|Q_{\boldsymbol{\omega}}(\lambda) - U\chi_{[0,\infty)}(\lambda)|\,\mathrm{d}\lambda \leqslant \frac{1}{2}\int_{\mathbb{R}^{2d}} |\boldsymbol{\omega}\cdot\boldsymbol{z}'|^2 |W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.$$

Proof. Set $T(\lambda) := Q_{\boldsymbol{\omega}}(\lambda) - U\chi_{[0,\infty)}(\lambda)$. For $\lambda > 0$ we have

$$T(\lambda) = Q_{\boldsymbol{\omega}}(\lambda) - U = -\int_{\mathbb{R}^{2d}} \chi(\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda) W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',$$
$$T(-\lambda) = Q_{\boldsymbol{\omega}}(-\lambda) = \int_{\mathbb{R}^{2d}} \chi(-\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda) W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'.$$

Thus for $\lambda > 0$ we have

$$T(\lambda) + T(-\lambda) = \int_{\mathbb{R}^{2d}} \Big(\chi(-\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda) - \chi(\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda)\Big) W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',$$
$$|T(\lambda)| + |T(-\lambda)| \leqslant \int_{\mathbb{R}^{2d}} \chi(|\boldsymbol{\omega}\cdot\boldsymbol{z}'| \geqslant \lambda) |W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.$$

Integrating over $\lambda \in [0,\infty)$ and noting that

$$\int_0^\infty \Big(\chi(-\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda) - \chi(\boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant \lambda)\Big)\,\mathrm{d}\lambda = \begin{cases} \int_0^{-\boldsymbol{\omega}\cdot\boldsymbol{z}'} \mathrm{d}\lambda = -\boldsymbol{\omega}\cdot\boldsymbol{z}' & \text{if } \boldsymbol{\omega}\cdot\boldsymbol{z}' < 0, \\ -\int_0^{\boldsymbol{\omega}\cdot\boldsymbol{z}'} \mathrm{d}\lambda = -\boldsymbol{\omega}\cdot\boldsymbol{z}' & \text{if } \boldsymbol{\omega}\cdot\boldsymbol{z}' \geqslant 0, \end{cases}$$
$$\int_0^\infty \chi(|\boldsymbol{\omega}\cdot\boldsymbol{z}'| \geqslant \lambda)\,\mathrm{d}\lambda = |\boldsymbol{\omega}\cdot\boldsymbol{z}'|,$$
$$\int_0^\infty \lambda\,\chi(|\boldsymbol{\omega}\cdot\boldsymbol{z}'| \geqslant \lambda)\,\mathrm{d}\lambda = \tfrac{1}{2}|\boldsymbol{\omega}\cdot\boldsymbol{z}'|^2,$$

gives the stated result. □

One use of the above result is that it allows us to see that the boundary term A_1 is indeed well defined, as referred to in Remark 5.2.2.

Lemma 5.8.2. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ with integral equal to* 1*. Denote*

$$Q_{\max} := \sup_{\boldsymbol{\omega}\in\mathbb{S}^{2d-1}} \sup_{\lambda\in\mathbb{R}} |Q_{\boldsymbol{\omega}}(\lambda)|,$$

which in particular satisfies $1 \leqslant Q_{\max} \leqslant \int_{\mathbb{R}^{2d}} |W(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}$. Let $a \in L^1(\partial\Omega)$. Then the integrand in A_1

is absolutely integrable and satisfies the bound

$$|A_1(a,\Omega,f;W)| \leqslant \frac{2}{(2\pi)^d}\|a\|_{L^1(\partial\Omega)}\int_{\mathbb{R}^{2d}}|\boldsymbol{z}'W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}' \sup_{|t|\leqslant Q_{\max}\|a\|_{L^\infty(\partial\Omega)}}|f'(t)|.$$

Proof. First note that, since $f(0)=0$, we have

$$f(\chi_{[0,\infty)}(\lambda)a(\boldsymbol{u})) = \chi_{[0,\infty)}(\lambda)f(a(\boldsymbol{u})).$$

Therefore we have

$$\begin{aligned}
|A_1| &\leqslant \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}\Big|f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)a(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(a(\boldsymbol{u}))\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\leqslant \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}\Big|f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)a(\boldsymbol{u})) - f(\chi_{[0,\infty)}(\lambda)a(\boldsymbol{u}))\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\quad + \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}\Big|\chi_{[0,\infty)}(\lambda)f(a(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(a(\boldsymbol{u}))\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\leqslant \frac{1}{(2\pi)^d}\|f'\|_{L^\infty}\int_{\partial\Omega}\int_{\mathbb{R}}|a(\boldsymbol{u})||Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)-\chi_{[0,\infty)}(\lambda)|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\quad + \frac{1}{(2\pi)^d}\|f'\|_{L^\infty}\int_{\partial\Omega}\int_{\mathbb{R}}|a(\boldsymbol{u})||Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)-\chi_{[0,\infty)}(\lambda)|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}),
\end{aligned}$$

and applying Lemma 5.8.1 gives the stated bound. □

Another application of Lemma 5.8.1 is the following lemma, which allows us to write the boundary term A_1 in an alternative form in some special cases. This is used in the proof the eigenvalue counting function result, Corollary 5.3.1.

Lemma 5.8.3. *Let $W\in\mathscr{S}(\mathbb{R}^{2d})$ satisfy $\int_{\mathbb{R}^{2d}}W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}=1$, and denote*

$$\tilde{A}_1(a,\Omega,f;W) := \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}\Big(f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)a(\boldsymbol{u})) - \chi_{[0,\infty)}(\lambda)f(a(\boldsymbol{u}))\Big)\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}).$$

If a is constant or W is spherically symmetric then $A_1=\tilde{A}_1$.

Proof. By Lemma 5.8.1 we have

$$\begin{aligned}
\tilde{A}_1(a,\Omega,f;W) - A_1(a,\Omega,f;W) &= \frac{1}{(2\pi)^d}\int_{\partial\Omega}\int_{\mathbb{R}}f(a(\boldsymbol{u}))\Big(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)-\chi_{[0,\infty)}(\lambda)\Big)\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&= -\frac{1}{(2\pi)^d}\int_{\partial\Omega}f(a(\boldsymbol{u}))\,\boldsymbol{n}(\boldsymbol{u})\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\cdot\int_{\mathbb{R}^{2d}}\boldsymbol{z}'W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'\\
&= \frac{1}{(2\pi)^d}\int_{\Omega}\nabla_{\boldsymbol{z}}\big(f(a(\boldsymbol{z}))\big)\,\mathrm{d}\boldsymbol{z}\cdot\int_{\mathbb{R}^{2d}}\boldsymbol{z}'W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}'.
\end{aligned}$$

When W is spherically symmetric the $\mathrm{d}\boldsymbol{z}'$ integral is zero, and when a is constant on Ω the integrand $\nabla_{\boldsymbol{z}}(f(a(\boldsymbol{z}))$ is identically zero. □

Chapter 6

Proof of result

In this chapter we prove the main result, described in §5.2: the Szegő theorem for $T_r[a\chi_\Omega]$. We also prove the Szegő theorem for the class of examples with a cusp boundary described in §5.6.

To avoid dealing with the scaling parameter r throughout the whole proof, we will give names to the rescaled versions of a and Ω. We write

$$T_r[a\chi_\Omega] = \operatorname{op}[W*(b\chi_\Sigma)], \qquad \text{where } b := a(\cdot/r),\ \Sigma := r\Omega.$$

The theorem will be proved in terms of general b, Σ without explicit reference to the fact that they are rescaled versions of other objects. However, in each step the remainder scales in such a way that it is $O(r^{2d-2})$ when b and Σ are of this form.

There are two variants of the theorem, Theorem 5.2.6 for C^2 boundary and Theorem 5.2.8 for compact non-smooth boundary, but their proofs have the same overall structure of two steps. The first step is composition. This says that

$$f(\operatorname{op}[W*(b\chi_\Sigma)]) \approx \operatorname{op}[f(W*(b\chi_\Sigma))],$$

where the approximation holds in the sense that the trace norm of the difference is of the correct asymptotic order. The general idea behind the proof of this is discussed in §5.7.

Combined with the fact that $|\operatorname{tr} A| \leqslant \|A\|_1$ for every trace class operator A, the composition step tells us that

$$\operatorname{tr} f(T_r[a\chi_\Omega]) = \operatorname{tr}\operatorname{op}[f(W*(b\chi_\Sigma))] + O(r^{2d-2}).$$

The trace is given by the integral of the Weyl symbol (Lemma 2.1.3), so (using the fact that $f(\chi_\Sigma b) = \chi_\Sigma f(b)$) we have

$$\begin{aligned}\operatorname{tr}\operatorname{op}[f(W*(b\chi_\Sigma))] &= \int_{\mathbb{R}^{2d}} f(W*(b\chi_\Sigma)(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} \\ &= \int_{\mathbb{R}^{2d}} W*(f(b\chi_\Sigma))(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} + \int_{\mathbb{R}^{2d}} \Big(f(W*(\chi_\Sigma b)(\boldsymbol{z})) - W*(\chi_\Sigma f(b))(\boldsymbol{z})\Big)\,\mathrm{d}\boldsymbol{z}.\end{aligned}$$

By Lemma 5.1.2 (second part), the first term is simply $A_0(b,\Sigma,f)$, which equals $r^{2d}A_0(a,\Omega,f)$. The second term is very similar to $A_1(b,\Sigma,f;W)$; in particular its integrand is concentrated near to $\partial\Sigma$. However, unlike A_1, it is not of the correct asymptotic form; it is not r^{2d-1} multiplied by its unscaled version. The second step of the proof is to use the local geometry of $\partial\Sigma$ (in particular the geometrical facts in §4.6) to show that this integral is indeed approximately equal to A_1.

The first two sections, §6.1 and §6.2, contain the proof of the two respective steps described above for Theorem 5.2.6, where the boundary of Ω is C^2. In §6.3 we prove an extra geometrical property needed for the non-smooth case: that, because Ω is a Lipschitz domain, we may conclude there are no cusps between the pieces making up the boundary. The following two sections, §6.4 and §6.5, contain the proof of the two respective steps for Theorem 5.2.8, where the boundary of Ω may be non-smooth. Finally, in §6.6, we prove the class of examples with a cusp in the boundary, as described in §5.6.

6.1 Composition for smooth boundary

In this section we prove Lemma 6.1.1, which as described at the start of this chapter is the first step in proving Theorem 5.2.6.

Lemma 6.1.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ satisfy $\int W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, let W, b, Σ, f satisfy Condition 5.2.3 and Condition 5.2.4, and let $\partial\Sigma$ have tubular radius of at least* 1*. Then there exists R such that*

$$\left\| f\big(\mathrm{op}[W*(b\chi_\Sigma)]\big) - \mathrm{op}\big[f(W*(b\chi_\Sigma))\big]\right\|_1 \leqslant R(b,\Sigma;W,f),$$

where R satisfies the scaling property

$$R(b,\Sigma;W,f) = r^{2d-2}R(a,\Omega;W,f), \qquad \text{for } b = a(\cdot/r),\ \Sigma = r\Omega.$$

Proof. Summary. Set $G := 2d+2$, $D := G+4d+2$, and apply Lemma 3.4.3 with $q := W*(b\chi_\Sigma)$. First note that (using Notation 3.4.1) by Lemma 5.1.2 we have

$$\mathsf{N}^D_\infty(W*(b\chi_\Sigma)) = \sum_{|\boldsymbol{m}|\leqslant D} \|(\partial^{\boldsymbol{m}} W)*(b\chi_\Sigma)\|_{L^\infty(\mathbb{R}^{2d})} \lesssim \|b\|_{L^\infty(\Sigma)}.$$

It thus remains to bound $\mathsf{M}^{G,D}(F_1)$; indeed, we will show that

$$\mathsf{M}^{G,D}(F_1) \lesssim \|\nabla b\|_{L^\infty(\Sigma)}(\|\nabla b\|_{L^1(\Sigma)} + \|b\|_{L^1(\partial\Sigma)}) + \frac{1}{\tau(\partial\Sigma)}\|b\|_{L^\infty(\partial\Sigma)}\|b\|_{L^1(\partial\Sigma)},$$

which has the required scaling property.

Expansion of differential operator. We have

$$\begin{aligned} F_1(\boldsymbol{x},\boldsymbol{y}) &= \frac{\mathrm{i}}{2}(\nabla_{\boldsymbol{x}_1}\cdot\nabla_{\boldsymbol{y}_2} - \nabla_{\boldsymbol{x}_2}\cdot\nabla_{\boldsymbol{y}_1})(W*(b\chi_\Sigma)(\boldsymbol{x})W*(b\chi_\Sigma)(\boldsymbol{y})) \\ &= \frac{\mathrm{i}}{2}\sum_{j=1}^{d}\big(\partial_{(\boldsymbol{x}_1)_j}\partial_{(\boldsymbol{y}_2)_j} - \partial_{(\boldsymbol{x}_2)_j}\partial_{(\boldsymbol{y}_1)_j}\big)(W*(b\chi_\Sigma)(\boldsymbol{x})W*(b\chi_\Sigma)(\boldsymbol{y})). \end{aligned}$$

For $j \in \{1,\dots,d\}$ we have

$$\partial_{(z_1)_j} W*(b\chi_\Sigma)(z) = g_{1,j}(z) + h_{1,j}(z),$$

where

$$g_{1,j}(z) := \int_{\partial\Sigma} W(z-z')b(z')(n_1)_j(z')\,\mathrm{d}z', \quad h_{1,j}(z) := W*(\chi_\Sigma\,\partial_{(z_1)_j} b)(z),$$

and similarly for $\partial_{(z_2)_j} W*(b\chi_\Sigma)(z)$. Thus, using the symmetry and subadditivity of $\mathsf{M}(\cdot)$, we have

$$\begin{aligned}\mathsf{M}^{G,D}(F_1) \leqslant \frac{1}{2}\sum_{j=1}^{d}\Big(&\mathsf{M}^{G,D}(g_{1,j}(x)g_{2,j}(y) - g_{2,j}(x)g_{1,j}(y))\\ &+2\mathsf{M}^{G,D}(g_{1,j}(x)h_{2,j}(y)) + 2\mathsf{M}^{G,D}(g_{2,j}(x)h_{1,j}(y)) + 2\mathsf{M}^{G,D}(h_{1,j}(x)h_{2,j}(y))\Big).\end{aligned}$$

<u>Terms involving $h_{1,j}$ or $h_{2,j}$.</u> To bound these terms we will use the facts

$$\begin{aligned}\mathsf{N}_1^D(g_{1,j}) &\leqslant \sum_{|k|\leqslant D}\int_{\mathbb{R}^{2d}}\int_{\partial\Sigma}|\partial^k W(z-z')||b(z')|\,\mathrm{d}z'\,\mathrm{d}z \lesssim \|b\|_{L^1(\partial\Sigma)},\\ \mathsf{N}_\infty^D(h_{1,j}) &\leqslant \sum_{|k|\leqslant D}\sup_{z\in\mathbb{R}^{2d}}\int_{\Sigma}|\partial^k W(z-z')||\partial_{(z_1')_j} b(z')|\,\mathrm{d}z' \lesssim \|\nabla b\|_{L^\infty(\Sigma)},\\ \mathsf{N}_1^D(h_{1,j}) &\leqslant \sum_{|k|\leqslant D}\int_{\mathbb{R}^{2d}}\int_{\Sigma}|\partial^k W(z-z')||\partial_{(z_1')_j} b(z')|\,\mathrm{d}z'\,\mathrm{d}z \lesssim \|\nabla b\|_{L^1(\Sigma)},\end{aligned}$$

as in Lemma 5.1.2, and similarly for $g_{2,j}$ and $h_{2,j}$. By Lemma 3.4.2 we thus have

$$\begin{aligned}\mathsf{M}^{G,D}(g_{1,j}(x)h_{2,j}(y)) &\lesssim \mathsf{N}_1^D(g_{1,j})\mathsf{N}_\infty^D(h_{2,j}) \lesssim \|b\|_{L^1(\partial\Sigma)}\|\nabla b\|_{L^\infty(\Sigma)},\\ \mathsf{M}^{G,D}(g_{2,j}(x)h_{1,j}(y)) &\lesssim \mathsf{N}_1^D(g_{2,j})\mathsf{N}_\infty^D(h_{1,j}) \lesssim \|b\|_{L^1(\partial\Sigma)}\|\nabla b\|_{L^\infty(\Sigma)},\\ \mathsf{M}^{G,D}(h_{1,j}(x)h_{2,j}(y)) &\lesssim \mathsf{N}_1^D(h_{1,j})\mathsf{N}_\infty^D(h_{2,j}) \lesssim \|\nabla b\|_{L^1(\Sigma)}\|\nabla b\|_{L^\infty(\Sigma)}.\end{aligned}$$

<u>Bound for first term.</u> First note that

$$g_{1,j}(x)g_{2,j}(y) - g_{2,j}(x)g_{1,j}(y) = \int_{\partial\Sigma}\int_{\partial\Sigma} W(x-x')b(x')W(y-y')b(y')m(x',y')\,\mathrm{d}x'\,\mathrm{d}y',$$

where for each $x', y' \in \partial\Sigma$ we denote

$$\begin{aligned}m(x',y') &:= (n_1)_j(x')(n_2)_j(y') - (n_2)_j(x')(n_1)_j(y')\\ &= \big((n_1)_j(x') - (n_1)_j(y')\big)(n_2)_j(y') + \big((n_2)_j(y') - (n_2)_j(x')\big)(n_1)_j(y').\end{aligned}$$

Let $\ell(x',y')$ be the line segment connecting x' to y'. When $|x'-y'| \leqslant \frac{1}{2}\tau(\partial\Sigma)$ we have $\ell(x',y') \subseteq \mathrm{tub}_{\tau(\partial\Omega)/2}(\partial\Sigma)$ so by Lemma 4.6.3 (using the extension of n defined in Notation 4.3.6) we have

$$\big|(n_1)_j(x') - (n_1)_j(y')\big| \leqslant |x'-y'|\sup_{z\in\ell(x',y')}|\nabla\otimes n(z)| \leqslant \frac{2|x'-y'|}{\tau(\partial\Sigma)}.$$

When $|\boldsymbol{x}'-\boldsymbol{y}'| \geqslant \frac{1}{2}\tau(\partial\Sigma)$ we have

$$\left|(\boldsymbol{n}_1)_j(\boldsymbol{x}')-(\boldsymbol{n}_1)_j(\boldsymbol{y}')\right| \leqslant 2 \leqslant \frac{4|\boldsymbol{x}'-\boldsymbol{y}'|}{\tau(\partial\Sigma)}.$$

Similar bounds hold for $\boldsymbol{n}_2$, so

$$|\boldsymbol{m}(\boldsymbol{x}',\boldsymbol{y}')| \leqslant \frac{8|\boldsymbol{x}'-\boldsymbol{y}'|}{\tau(\partial\Sigma)},$$

which we may combine with the fact that

$$|\boldsymbol{x}'-\boldsymbol{y}'| \leqslant |\boldsymbol{x}-\boldsymbol{x}'|+|\boldsymbol{x}-\boldsymbol{y}|+|\boldsymbol{y}-\boldsymbol{y}'| \leqslant 3\langle \boldsymbol{x}-\boldsymbol{x}'\rangle\langle \boldsymbol{x}-\boldsymbol{y}\rangle\langle \boldsymbol{y}-\boldsymbol{y}'\rangle.$$

We also bound (using Lemma 4.6.6 with $V(\boldsymbol{z}) := \langle \boldsymbol{z}\rangle|\partial^{\boldsymbol{l}} W(\boldsymbol{z})|$ for the $\mathrm{d}\boldsymbol{x}'$ integral and just bounding by $\psi_V(0)$)

$$\int_{\partial\Sigma} \langle \boldsymbol{x}-\boldsymbol{x}'\rangle|\partial^{\boldsymbol{l}} W(\boldsymbol{x}-\boldsymbol{x}')b(\boldsymbol{x}')|\,\mathrm{d}\boldsymbol{x}' \lesssim \|b\|_{L^\infty(\partial\Sigma)},$$
$$\int_{\mathbb{R}^{2d}}\int_{\partial\Sigma} \langle \boldsymbol{y}-\boldsymbol{y}'\rangle|\partial^{\boldsymbol{m}} W(\boldsymbol{y}-\boldsymbol{y}')b(\boldsymbol{y}')|\,\mathrm{d}\boldsymbol{y}'\,\mathrm{d}\boldsymbol{y} \lesssim \|b\|_{L^1(\partial\Sigma)}.$$

We therefore obtain

$$\mathsf{M}^{G,D}(g_{1,j}(\boldsymbol{x})g_{2,j}(\boldsymbol{y})-g_{2,j}(\boldsymbol{x})g_{1,j}(\boldsymbol{y})) \lesssim \frac{\|b\|_{L^\infty(\partial\Sigma)}\|b\|_{L^1(\partial\Sigma)}}{\tau(\partial\Sigma)}. \qquad \square$$

6.2 Trace asymptotics for smooth boundary

In this section we prove Lemma 6.2.1, which as discussed at the start of this chapter completes the proof of Theorem 5.2.6.

Lemma 6.2.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ satisfy $\int W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, and let W, b, Σ, f satisfy Condition 5.2.3 and Condition 5.2.4. Then there exists R such that, using Notation 3.4.1, we have*

$$\left|\int_{\mathbb{R}^{2d}} f(W*(b\chi_\Sigma)(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} - \Big(A_0(b,\Sigma,f)+A_1(b,\Sigma,f;W)\Big)\right| \leqslant R(b,\Sigma;W,f),$$

where R satisfies the scaling property

$$R(b,\Sigma;W,f) = r^{2d-2}R(a,\Omega;W,f), \qquad \text{for } b = a(\cdot/r),\ \Sigma = r\Omega.$$

Notation 6.2.2. In this section we will refer to the tubular radius of the boundary of Σ very often, so instead of using the full notation $\tau(\partial\Sigma)$ we will refer to it simply as τ (which for $\Sigma = r\Omega$ equals $r\tau(\partial\Omega)$).

Proof of Lemma 6.2.1. Summary. Denote

$$I_1 := \int_{\mathbb{R}^{2d}} \Big(f(W*(\chi_\Sigma b)(\boldsymbol{z})) - W*(\chi_\Sigma f(b))(\boldsymbol{z})\Big)\,\mathrm{d}\boldsymbol{z},$$
$$I_5 := \int_{\partial\Sigma}\int_{\mathbb{R}} \Big(f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)b(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(b(\boldsymbol{u}))\Big)\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}).$$

We must show that when $b = a(\cdot/r)$ and $\Sigma = r\Omega$, we have $I_1 = I_5 + O(r^{2d-2})$, as explained at the start of this chapter (because I_5 is the asymptotic term A_1, and I_1 is the term discussed there). To do this, we will begin by noticing that it suffices to consider f and W that are compactly supported. Then we will observe a chain of approximations starting with I_1 and finishing with I_5.

Step 1: Restrict support of f. Depending on which part of Condition 5.2.3 is satisfied, either f is a smooth function on $\mathbb{R}$, while b, W are real-valued, or f is a smooth function on $\mathbb{C}$. In both cases, I_1 and I_5 only depend on the value of $f(t)$ for

$$|t| \leqslant \|b\|_{L^\infty(\Sigma)} \int_{\mathbb{R}^{2d}} |W(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z},$$

so we may restrict the support of f to a compact set, and when b and Σ scale in the stated way this set does not depend on r. In the remainder of the proof we refer to $\|f\|_{L^\infty}$ for the supremum of $|f|$ over that set, and similarly for $\|f'\|_{L^\infty}$ and $\|f''\|_{L^\infty}$.

Step 2: Restrict support of W. In this step we restrict the support of W to $B_{\tau/2}(\mathbf{0})$. This change is asymptotically very small because the radius of support $\frac{1}{2}\tau$ is large. However, it will be useful in later steps because it will cause certain integrals to be zero outside of $\mathrm{tub}_{\tau/2}(\partial\Sigma)$, which will allow us to apply the results in Chapter 4 to bound them.

Let $\widetilde{W}$ be the function defined for each $\boldsymbol{z} \in \mathbb{R}^{2d}$ by

$$\widetilde{W}(\boldsymbol{z}) := \begin{cases} W(\boldsymbol{z}) + K_{W,\tau} & \text{if } |\boldsymbol{z}| \leqslant \frac{1}{2}\tau, \\ 0 & \text{if } |\boldsymbol{z}| > \frac{1}{2}\tau, \end{cases}$$

with $K_{W,\tau}$ chosen so that the integral of $\widetilde{W}$ is 1. Specifically, we set

$$K_{W,\tau} = \frac{1}{V(\tau,d)} \int_{|\boldsymbol{z}'|>\tau/2} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',$$

where $V(\tau,d) := \mu_{2d}(B(\mathbf{0},\tau/2)) = \mu_{2d}(B(\mathbf{0},1))(\tau/2)^{2d}$. Then

$$\begin{aligned}
\int_{\mathbb{R}^{2d}} \widetilde{W}(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' &= \int_{|\boldsymbol{z}'|<\tau/2} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' + \int_{|\boldsymbol{z}'|<\tau/2} K_{W,\tau}\,\mathrm{d}\boldsymbol{z}' \\
&= \int_{|\boldsymbol{z}'|<\tau/2} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' + \frac{V(\tau,d)}{V(\tau,d)} \int_{|\boldsymbol{z}'|>\tau/2} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' \\
&= \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' = 1.
\end{aligned}$$

The error in replacing W by $\widetilde{W}$ in I_1 satisfies (using Lemma 5.1.5 to bound $|f(b(\boldsymbol{z}))|$)

$$\begin{aligned}
|I_1 - \tilde{I}_1| &\leqslant \|f'\|_{L^\infty} \int |(W - \widetilde{W}) * (\chi_\Sigma b)(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} + \int |(W - \widetilde{W}) * (\chi_\Sigma f(b))(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} \\
&\leqslant 2\|f'\|_{L^\infty} \|b\|_{L^1(\Sigma)} \int_{\mathbb{R}^{2d}} |W(\boldsymbol{z}) - \widetilde{W}(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} \\
&\leqslant 4\|f'\|_{L^\infty} \|b\|_{L^1(\Sigma)} \int_{|\boldsymbol{z}'|\geqslant\tau/2} |W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.
\end{aligned}$$

Since $W \in \mathscr{S}(\mathbb{R}^{2d})$ this integral can be bounded by any negative power of τ; choosing to bound it by $1/\tau^2$ suffices to satisfy the required scaling property.

The error in replacing W by $\widetilde{W}$ in I_5 satisfies

$$
\begin{aligned}
|I_5-\tilde{I}_5| &\leqslant \|f'\|_{L^\infty}\int_{\partial\Sigma}\int_{\mathbb{R}}\Big|(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)-\widetilde{Q}_{\boldsymbol{n}(\boldsymbol{u})}(\lambda))b(\boldsymbol{u})\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\quad+\int_{\partial\Sigma}\int_{\mathbb{R}}\Big|(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)-\widetilde{Q}_{\boldsymbol{n}(\boldsymbol{u})}(\lambda))f(b(\boldsymbol{u}))\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\
&\leqslant 2\|f'\|_{L^\infty}\|b\|_{L^1(\partial\Sigma)}\sup_{\boldsymbol{\omega}\in\mathbb{S}^{2d-1}}\int_{\mathbb{R}}|Q_{\boldsymbol{\omega}}(\lambda)-\widetilde{Q}_{\boldsymbol{\omega}}(\lambda)|\,\mathrm{d}\lambda.
\end{aligned}
$$

Denote

$$
W_1(\boldsymbol{z}):=W(\boldsymbol{z})\chi(|\boldsymbol{z}|>\tfrac{1}{2}\tau),\quad W_2(\boldsymbol{z}):=K_{W,\tau}\chi(|\boldsymbol{z}|\leqslant\tfrac{1}{2}\tau),
$$

so that $W-\widetilde{W}=W_1-W_2$. Set $U:=\int_{|\boldsymbol{z}|>\tau/2}W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}$; note that the integrals of both W_1 and of W_2 equal U. Then

$$
\begin{aligned}
Q_{\boldsymbol{\omega}}(\lambda)-\widetilde{Q}_{\boldsymbol{\omega}}(\lambda) &= \int_{\{\boldsymbol{z}'\in\mathbb{R}^{2d}:\boldsymbol{z}'\cdot\boldsymbol{\omega}\leqslant\lambda\}}(W(\boldsymbol{z}')-\widetilde{W}(\boldsymbol{z}'))\,\mathrm{d}\boldsymbol{z}'\\
&= \int_{\{\boldsymbol{z}'\in\mathbb{R}^{2d}:\boldsymbol{z}'\cdot\boldsymbol{\omega}\leqslant\lambda\}}(W_1(\boldsymbol{z}')-W_2(\boldsymbol{z}'))\,\mathrm{d}\boldsymbol{z}'\\
&= Q_{1,\boldsymbol{\omega}}(\lambda)-Q_{2,\boldsymbol{\omega}}(\lambda)\\
&= (Q_{1,\boldsymbol{\omega}}(\lambda)-U\chi_{[0,\infty)}(\lambda))-(Q_{2,\boldsymbol{\omega}}(\lambda)-U\chi_{[0,\infty)}(\lambda)),
\end{aligned}
$$

where $Q_{1,\boldsymbol{\omega}},Q_{2,\boldsymbol{\omega}}$ are the $Q_{\boldsymbol{\omega}}$ corresponding to W_1,W_2 respectively. Applying Lemma 5.8.1 gives

$$
\begin{aligned}
|I_5-\tilde{I}_5| &\leqslant 2\|f'\|_{L^\infty}\|b\|_{L^1(\partial\Sigma)}\Big(\int_{\mathbb{R}^{2d}}|\boldsymbol{z}'W_1(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'+\int_{\mathbb{R}^{2d}}|\boldsymbol{z}'W_2(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\Big)\\
&\leqslant 4\|f'\|_{L^\infty}\|b\|_{L^1(\partial\Sigma)}\int_{|\boldsymbol{z}|>\tau/2}|\boldsymbol{z}'||W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.
\end{aligned}
$$

As before, this may be bounded by any negative power of τ; choosing to bound it by $1/\tau$ suffices. This completes the proof that we may restrict W to have support in $B_{\tau/2}(\mathbf{0})$.

We will now show that any bound depending suitably on an integral of $\widetilde{W}$ may replaced by one depending on W uniformly in τ; specifically, for each $k\in\mathbb{N}_0$,

$$
\int_{\mathbb{R}^{2d}}(1+|\boldsymbol{z}'|)^k|\widetilde{W}(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\leqslant\int_{\mathbb{R}^{2d}}(1+|\boldsymbol{z}'|)^k|W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'.
$$

To see this, note that

$$
\int_{\mathbb{R}^{2d}}(1+|\boldsymbol{z}|)^k|\widetilde{W}(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}\leqslant\int_{|\boldsymbol{z}|<\tau/2}(1+|\boldsymbol{z}|)^k|W(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}+\int_{|\boldsymbol{z}|<\tau/2}(1+|\boldsymbol{z}|)^k|K_{W,\tau}|\,\mathrm{d}\boldsymbol{z}.
$$

The second term is

$$
\begin{aligned}
\int_{|\boldsymbol{z}|<\tau/2}(1+|\boldsymbol{z}|)^k|K_{W,\tau}|\,\mathrm{d}\boldsymbol{z} &\leqslant \frac{1}{V(\tau,d)}\int_{|\boldsymbol{z}|<\tau/2}\int_{|\boldsymbol{z}'|>\tau/2}(1+|\boldsymbol{z}|)^k|W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\,\mathrm{d}\boldsymbol{z}\\
&\leqslant \frac{1}{V(\tau,d)}\Big(\int_{|\boldsymbol{z}|<\tau/2}\mathrm{d}\boldsymbol{z}\Big)\Big(\int_{|\boldsymbol{z}'|>\tau/2}(1+|\boldsymbol{z}'|)^k|W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\Big),
\end{aligned}
$$

and the integrand in the first bracket equals $V(\tau,d)$, so the bound takes the stated form. For the rest of the proof we use $\widetilde{W}$ (and $\tilde{I}_1$, $\tilde{I}_5$) in place of W (and I_1, I_5 resp.) without further comment.

Step 3: Extract b from convolution. Let

$$I_2 := \int_{\mathbb{R}^{2d}} \Big(f(W * \chi_\Sigma(\boldsymbol{z}) b(\boldsymbol{z})) - W * \chi_\Sigma(\boldsymbol{z}) f(b(\boldsymbol{z})) \Big) \,\mathrm{d}\boldsymbol{z}.$$

We will bound $|I_1 - I_2|$. We can rewrite $I_1 - I_2 = \int_{\mathbb{R}^{2d}} (D_1(\boldsymbol{z}) - D_2(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z}$, where

$$\begin{aligned} D_1(\boldsymbol{z}) &:= f(W * (\chi_\Sigma b)(\boldsymbol{z})) - f(W * \chi_\Sigma(\boldsymbol{z}) b(\boldsymbol{z})), \\ D_2(\boldsymbol{z}) &:= W * (\chi_\Sigma f(b))(\boldsymbol{z}) - W * \chi_\Sigma(\boldsymbol{z}) f(b(\boldsymbol{z})). \end{aligned}$$

We use the two-term Taylor's theorem with integral remainder; that is, for any sufficiently smooth function p,

$$\begin{aligned} &W * (\chi_\Omega p)(\boldsymbol{z}) - W * \chi_\Omega(\boldsymbol{z}) p(\boldsymbol{z}) \\ &\quad = \int_{\mathbb{R}^{2d}} W(\boldsymbol{z}') \chi_\Omega(\boldsymbol{z} - \boldsymbol{z}')(-\boldsymbol{z}' \cdot \nabla) p(\boldsymbol{z}) \,\mathrm{d}\boldsymbol{z}' \\ &\qquad + \int_0^1 \int_{\mathbb{R}^{2d}} (1-t) W(\boldsymbol{z}') \chi_\Omega(\boldsymbol{z} - \boldsymbol{z}')(-\boldsymbol{z}' \cdot \nabla)^2 p(\boldsymbol{z} - t\boldsymbol{z}') \,\mathrm{d}\boldsymbol{z}' \,\mathrm{d}t. \end{aligned}$$

Applying this to b we have

$$D_1(\boldsymbol{z}) = f\Big(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z}) + (-\boldsymbol{z}' W(\boldsymbol{z}')) * \chi_\Omega(\boldsymbol{z}) \cdot \nabla b(\boldsymbol{z}) \Big) - f(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z})) + r_1(\boldsymbol{z}),$$

where

$$\begin{aligned} \int_{\mathbb{R}^{2d}} |r_1(\boldsymbol{z})| \,\mathrm{d}\boldsymbol{z} &\leqslant \|f'\|_{L^\infty} \int_{\mathbb{R}^{2d}} \int_0^1 \int_{\mathbb{R}^{2d}} (1-t) \Big| W(\boldsymbol{z}') \chi_\Omega(\boldsymbol{z} - \boldsymbol{z}')(\boldsymbol{z}' \cdot \nabla)^2 b(\boldsymbol{z} - t\boldsymbol{z}') \Big| \,\mathrm{d}\boldsymbol{z}' \,\mathrm{d}t \,\mathrm{d}\boldsymbol{z} \\ &\leqslant \|f'\|_{L^\infty} \int_{\mathbb{R}^{2d}} |\boldsymbol{z}'|^2 |W(\boldsymbol{z}')| \,\mathrm{d}\boldsymbol{z}' \int_{\mathbb{R}^{2d}} |\nabla \otimes \nabla b(\boldsymbol{z})| \,\mathrm{d}\boldsymbol{z} \\ &\lesssim \|f'\|_{L^\infty} \|\nabla \otimes \nabla b\|_{L^1(\mathbb{R}^{2d})}. \end{aligned}$$

But applying Taylor's theorem to f we obtain

$$\begin{aligned} &f\Big(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z}) + (-\boldsymbol{z}' W(\boldsymbol{z}')) * \chi_\Omega(\boldsymbol{z}) \cdot \nabla b(\boldsymbol{z}) \Big) \\ &\qquad = f(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z})) + (-\boldsymbol{z}' W(\boldsymbol{z}')) * \chi_\Omega(\boldsymbol{z}) \cdot \nabla b(\boldsymbol{z}) f'(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z})) + r_2(\boldsymbol{z}), \end{aligned}$$

where

$$\begin{aligned} \int_{\mathbb{R}^{2d}} |r_2(\boldsymbol{z})| \,\mathrm{d}\boldsymbol{z} &\leqslant \|f''\|_{L^\infty} \int_{\mathbb{R}^{2d}} \Big| (\boldsymbol{z}' W(\boldsymbol{z}')) * \chi_\Omega(\boldsymbol{z}) \cdot \nabla b(\boldsymbol{z}) \Big|^2 \,\mathrm{d}\boldsymbol{z} \\ &\lesssim \|f''\|_{L^\infty} \|\nabla b\|_{L^\infty(\mathbb{R}^{2d})} \|\nabla b\|_{L^1(\mathbb{R}^{2d})}. \end{aligned}$$

Thus

$$D_1(\boldsymbol{z}) = (-\boldsymbol{z}' W(\boldsymbol{z}')) * \chi_\Omega(\boldsymbol{z}) \cdot \nabla b(\boldsymbol{z}) f'(W * \chi_\Omega(\boldsymbol{z}) b(\boldsymbol{z})) + r_1(\boldsymbol{z}) + r_2(\boldsymbol{z}).$$

Applying the two term Taylor expansion to $f(b)$ we have

$$D_2(\boldsymbol{z}) = (-\boldsymbol{z}'W(\boldsymbol{z}'))*\chi_\Omega(\boldsymbol{z})\cdot\nabla b(\boldsymbol{z})f'(b(\boldsymbol{z}))+r_3(\boldsymbol{z}),$$

where

$$\begin{aligned}\int_{\mathbb{R}^{2d}}|r_3(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z} &\leqslant \int_{\mathbb{R}^{2d}}\int_0^1\int_{\mathbb{R}^{2d}}(1-t)\Big|W(\boldsymbol{z}')(\boldsymbol{z}'\cdot\nabla)^2(f(b))(\boldsymbol{z}-t\boldsymbol{z}')\Big|\,\mathrm{d}\boldsymbol{z}'\,\mathrm{d}t\,\mathrm{d}\boldsymbol{z}\\ &\leqslant \Big(\int_{\mathbb{R}^{2d}}|\boldsymbol{z}'|^2|W(\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\Big)\Big(\int_{\mathbb{R}^{2d}}|\nabla\otimes\nabla(f(b))(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}\Big)\\ &\lesssim \|f''\|_{L^\infty}\|\nabla b\|_{L^\infty(\mathbb{R}^{2d})}\|\nabla b\|_{L^1(\mathbb{R}^{2d})}+\|f'\|_{L^\infty}\|\nabla\otimes\nabla b\|_{L^1(\mathbb{R}^{2d})}.\end{aligned}$$

It thus remains to bound

$$\int_{\mathbb{R}^{2d}}\Big|(\boldsymbol{z}'W(\boldsymbol{z}'))*\chi_\Sigma(\boldsymbol{z})\cdot\nabla b(\boldsymbol{z})\big(f'(W*\chi_\Sigma(\boldsymbol{z})b(\boldsymbol{z}))-f'(b(\boldsymbol{z}))\big)\Big|\,\mathrm{d}\boldsymbol{z}.$$

This integrand is zero outside of $\operatorname{tub}_{\tau/2}(\partial\Sigma)$. Set $V(\boldsymbol{z}') := (1+|\boldsymbol{z}'|)|W(\boldsymbol{z}')|$. By Lemma 4.6.5 and Lemma 4.6.8, this integral is thus bounded by

$$\begin{aligned}&\|f''\|_{L^\infty}\int_{\operatorname{tub}_{\tau/2}(\partial\Sigma)}\Big|(\boldsymbol{z}'W(\boldsymbol{z}'))*\chi_\Sigma(\boldsymbol{z})\cdot\nabla b(\boldsymbol{z})W*\chi_{\Sigma^c}(\boldsymbol{z})b(\boldsymbol{z})\Big|\,\mathrm{d}\boldsymbol{z}\\ &\quad\leqslant \|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^{2d})}\int_{\operatorname{tub}_{\tau/2}(\partial\Sigma)}|V*\chi_\Sigma(\boldsymbol{z})V*\chi_{\Sigma^c}(\boldsymbol{z})\nabla b(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}\\ &\quad\lesssim \|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^{2d})}(\|\nabla b\|_{L^1(\partial\Sigma)}+\|\nabla\otimes\nabla b\|_{L^1(\mathbb{R}^{2d})}).\end{aligned}$$

<u>Step 4: Approximate b by its value on $\partial\Sigma$.</u> Let

$$I_3 := \int_{\operatorname{tub}_{\tau/2}(\partial\Sigma)}\Big(f(W*\chi_\Sigma(\boldsymbol{z})b(\boldsymbol{u}))-W*\chi_\Sigma(\boldsymbol{z})f(b(\boldsymbol{u}))\Big)\,\mathrm{d}\boldsymbol{z},$$

where for each $\boldsymbol{z}\in\operatorname{tub}_{\tau/2}(\partial\Sigma)$ we define $\boldsymbol{u} := (e^{-1}(\boldsymbol{z}))_1\in\partial\Sigma$ (i.e. the nearest point function; see Definition 4.2.2 and Remark 4.2.5). The integrand of I_2 is zero outside of $\boldsymbol{z}\in\operatorname{tub}_{\tau/2}(\partial\Sigma)$, so

$$I_2 - I_3 = \int_{\operatorname{tub}_{\tau/2}(\partial\Sigma)}\Big(h(W*\chi_\Omega(\boldsymbol{z}),b(\boldsymbol{z}))-h(W*\chi_\Omega(\boldsymbol{z}),b(\boldsymbol{u}))\Big)\,\mathrm{d}\boldsymbol{z},$$

where $h(x,y) := f(xy)-xf(y)$. But for any x, y_1, y_2 we have

$$|h(x,y_1)-h(x,y_2)| \leqslant |y_1-y_2|\sup_{y\in[y_1,y_2]}|xf'(xy)-xf'(y)| \leqslant \|f''\|_{L^\infty}|y_1-y_2||x||1-x|\sup_{y\in[y_1,y_2]}|y|,$$

so

$$|I_2-I_3| \leqslant \|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^{2d})}\int_{\operatorname{tub}_{\tau/2}(\partial\Sigma)}|b(\boldsymbol{z})-b(\boldsymbol{u})||W*\chi_\Omega(\boldsymbol{z})||W*\chi_{\Omega^c}(\boldsymbol{z})|\,\mathrm{d}\boldsymbol{z}.$$

By Lemma 4.6.5 and Lemma 4.6.8 (i.e. Taylor's theorem on b in the $\boldsymbol{n}(\boldsymbol{u})$ direction) and we therefore have

$$|I_2-I_3| \lesssim \|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^{2d})}(\|\nabla b\|_{L^1(\partial\Sigma)}+\|\nabla\otimes\nabla b\|_{L^1(\mathbb{R}^{2d})}).$$

Step 5: Approximate Σ locally by a half space. By Lemma 4.3.3 the integral from the previous step may be written as

$$I_3 = \int_{\partial\Sigma}\int_{-\tau/2}^{\tau/2}\Big(f(W*\chi_\Sigma(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))b(\boldsymbol{u})) - W*\chi_\Sigma(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))f(b(\boldsymbol{u}))\Big)\det(I-\lambda S^{\boldsymbol{u}})\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})$$

Let

$$I_4 := \int_{\partial\Sigma}\int_{-\tau/2}^{\tau/2}\Big(f(Q_{\boldsymbol{n}(\boldsymbol{z})}(\lambda)b(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(b(\boldsymbol{u}))\Big)\det(I-\lambda S^{\boldsymbol{u}})\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}).$$

By Lemma 4.6.1 we have

$$\begin{aligned}|I_3 - I_4| &\lesssim \|f'\|_{L^\infty}\int_{\partial\Sigma}\int_{-\tau/2}^{\tau/2}|b(\boldsymbol{u})|\Big|W*\chi_\Sigma(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u})\\ &\leqslant \|f'\|_{L^\infty}\|b\|_{L^1(\partial\Sigma)}\sup_{\boldsymbol{u}\in\partial\Sigma} J(\boldsymbol{u}),\end{aligned}$$

where for each $\boldsymbol{u}\in\partial\Omega$ we set

$$J(\boldsymbol{u}) := \int_{-\tau/2}^{\tau/2}\Big|W*\chi_\Sigma(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)\Big|\,\mathrm{d}\lambda.$$

We will show that $J(\boldsymbol{u})\lesssim 1/\tau$. We have

$$Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) = W*\chi_H(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})), \qquad H := \{\boldsymbol{z}'\in\mathbb{R}^{2d} : (\boldsymbol{z}'-\boldsymbol{u})\cdot\boldsymbol{n}(\boldsymbol{u})\geqslant 0\}.$$

So, denoting symmetric difference by Δ, we have

$$\begin{aligned}J(\boldsymbol{u}) &\leqslant \int_{-\tau/2}^{\tau/2}|W|*\chi_{\Sigma\Delta H}(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u}))\,\mathrm{d}\lambda\\ &= \int_{-\tau/2}^{\tau/2}\int_{\Sigma\Delta H}|W(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})-\boldsymbol{z}')|\,\mathrm{d}\boldsymbol{z}'\,\mathrm{d}\lambda.\end{aligned}$$

Let us write $\boldsymbol{z}' = \boldsymbol{u}+\boldsymbol{t}+\xi\boldsymbol{n}(\boldsymbol{u})$, where $\boldsymbol{t}\in T^{\boldsymbol{u}}$ and $\xi\in\mathbb{R}$. This integrand is non-zero only when $\boldsymbol{z}'\in\Sigma\Delta H$, and by Lemma 4.2.6 we have $\Sigma\Delta H\subseteq B_\tau(\boldsymbol{u}\pm\tau\boldsymbol{n}(\boldsymbol{u}))^{\mathrm{c}}$, so when $|\boldsymbol{z}'-\boldsymbol{u}|<\tau$ (so that $\boldsymbol{z}'$ is between the two balls) we have

$$|\xi|\leqslant \tau - \sqrt{\tau^2-|\boldsymbol{t}|^2}.$$

We will use the fact, proved below, that this implies that $|\xi|\leqslant|\boldsymbol{t}|^2/\tau$. But the integrand is non-zero only when $|\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})-\boldsymbol{z}'|<\tau/2$ and $|\lambda|<\tau/2$, so we always have $|\boldsymbol{z}'-\boldsymbol{u}|<\tau$. Thus

$$J(\boldsymbol{u})\leqslant\int_{-\tau/2}^{\tau/2}\int_{T^{\boldsymbol{u}}}\int_{-|\boldsymbol{t}|^2/\tau}^{|\boldsymbol{t}|^2/\tau}|W(\lambda\boldsymbol{n}(\boldsymbol{u})-\xi\boldsymbol{n}(\boldsymbol{u})-\boldsymbol{t})|\,\mathrm{d}\xi\,\mu_{2d-1}(\mathrm{d}\boldsymbol{t})\,\mathrm{d}\lambda.$$

Translating λ to $\eta:=\lambda-\xi$ we obtain

$$\begin{aligned}J(\boldsymbol{u}) &\leqslant \int_{T^{\boldsymbol{u}}}\int_{-|\boldsymbol{t}|^2/\tau}^{|\boldsymbol{t}|^2/\tau}\int_{\mathbb{R}}|W(\eta\boldsymbol{n}(\boldsymbol{u})-\boldsymbol{t})|\,\mathrm{d}\eta\,\mathrm{d}\xi\,\mu_{2d-1}(\mathrm{d}\boldsymbol{t})\\ &\leqslant \int_{T^{\boldsymbol{u}}}\int_{\mathbb{R}}\frac{2|\boldsymbol{t}|^2}{\tau}|W(\eta\boldsymbol{n}(\boldsymbol{u})-\boldsymbol{t})|\,\mathrm{d}\eta\,\mu_{2d-1}(\mathrm{d}\boldsymbol{t})\end{aligned}$$

and setting $\boldsymbol{x} := \eta\boldsymbol{n}(\boldsymbol{u}) - \boldsymbol{t}$ gives

$$J(\boldsymbol{u}) \leqslant \frac{2}{\tau}\int_{\mathbb{R}^{2d}} |\boldsymbol{x}|^2 |W(\boldsymbol{x})|\,\mathrm{d}\boldsymbol{x} \lesssim \frac{1}{\tau}.$$

Now we prove the claim made above that $|\xi| \leqslant |\boldsymbol{t}|^2/\tau$. First note that $|\boldsymbol{t}| \leqslant |\boldsymbol{z}' - \boldsymbol{u}| < \tau$. We trivially have $\tau^2 - |\boldsymbol{t}|^2 \leqslant \tau^2$, and because $|\boldsymbol{t}|^2 < \tau^2$ multiplying both sides of this by $\tau^2 - |\boldsymbol{t}|^2$ preserves the inequality, giving

$$(\tau^2 - |\boldsymbol{t}|^2)^2 \leqslant \tau^2(\tau^2 - |\boldsymbol{t}|^2).$$

Taking the square root of both sides (which are strictly positive) and rearranging gives

$$\tau - \sqrt{\tau^2 - |\boldsymbol{t}|^2} \leqslant \frac{|\boldsymbol{t}|^2}{\tau}.$$

But $|\xi|$ is bounded by the left hand side, so this implies that $|\xi| \leqslant |\boldsymbol{t}|^2/\tau$.

Step 6: Neglect Jacobian. In I_5 (see the start of this proof) the integrand is zero except for when $|\lambda| < \tau/2$, so using Lemma 4.6.2 to bound the Jacobian difference and Lemma 5.8.1 to bound the $\mathrm{d}\lambda$ integral, we have

$$\begin{aligned}
|I_4 - I_5| &\leqslant \int_{\partial\Sigma}\int_{\mathbb{R}} \Big| f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) b(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) f(b(\boldsymbol{u}))\Big| |\det(I - \lambda S^{\boldsymbol{u}}) - 1|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \\
&\lesssim \frac{1}{\tau}\int_{\partial\Sigma}\int_{-\tau/2}^{\tau/2} |\lambda| \Big| f(Q_{\boldsymbol{n}(\boldsymbol{z})}(\lambda) b(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda) f(b(\boldsymbol{u}))\Big|\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \\
&\leqslant \frac{2}{\tau}\|f'\|_{L^\infty}\int_{\partial\Sigma} |b(\boldsymbol{u})|\mu_{2d-1}(\mathrm{d}\boldsymbol{u}) \int_{\mathbb{R}} |\lambda| \Big| Q_{\boldsymbol{n}(\boldsymbol{z})}(\lambda) - \chi_{[0,\infty)}(\lambda)\Big|\,\mathrm{d}\lambda \\
&\lesssim \frac{1}{\tau}\|f'\|_{L^\infty}\|b\|_{L^1(\partial\Sigma)}.
\end{aligned}$$

□

6.3 Cusp-free property

We will need another geometrical fact before proving the Szegő theorem for domains with non-smooth boundaries. We will show that the domains in question have no cusps, in a sense that we will make precise in a moment.

The only relevant assumption here is that the domain is Lipschitz. For example, the graph $y = \sqrt{|x|}$ in $\mathbb{R}^2$, which is not Lipschitz, is piecewise C^∞ but still has a cusp. Indeed, this chapter makes no use at all of the tubular theory developed in Chapter 4, and until the end all results are just stated in terms of two closed sets $U, V \subseteq \partial\Omega$ such that $U \cup V = \partial\Omega$. For ease of application, we then express this in terms of the C^2 extensible pieces that comprise the boundary by choosing $U = \Gamma_i$ and $V = \bigcup_{j\neq i}\Gamma_j$. There is no novelty in noticing that Lipschitz domains have no cusps — that is the whole point of using Lipschitz domains — but the author was not able to find this fact expressed in precisely the way needed here.

We will view the idea of having "no cusp" in two ways, which may be expressed intuitively as follows:

1. If points $\boldsymbol{u} \in U$ and $\boldsymbol{v} \in V$ are both at least some small distance d from $U \cap V$ (considered as the corner between U and V) then the distance between $\boldsymbol{u}$ and $\boldsymbol{v}$ is at least proportional to d. This constant of proportionality is like the angle between U and V.

2. If we have a point $\boldsymbol{z} \in \mathbb{R}^m$ that is distant from the corner $U \cap V$ then it must be distant from one of the surfaces. This can be seen from the previous point by noting that if there were points $\boldsymbol{u} \in U$ and $\boldsymbol{v} \in V$ that were both close to $\boldsymbol{z}$ (compared to their distance from $U \cap V$), then it would follow that they would be close to each other, violating that condition.

The first of these two ideas is made explicit in the following condition. The lemma immediately afterwards shows that it holds for all Lipschitz domains.

Condition 6.3.1. Let $U, V \subseteq \mathbb{R}^m$ be closed sets for which there exists $k > 0$ and $\rho > 0$ such that

$$\forall \boldsymbol{u} \in U, \boldsymbol{v} \in V \text{ satisfying } |\boldsymbol{u} - \boldsymbol{v}| < k, \qquad \text{we have } \operatorname{dist}(\boldsymbol{u}, U \cap V) + \operatorname{dist}(\boldsymbol{v}, U \cap V) \leqslant \rho |\boldsymbol{u} - \boldsymbol{v}|.$$

Lemma 6.3.2. *Let $\Gamma \subseteq \mathbb{R}^m$ (for $m \geqslant 2$) be a closed bounded Lipschitz manifold of dimension $m-1$. Let $U, V \subseteq \Gamma$ be non-empty closed sets such that $U \cup V = \Gamma$. Then there exists $k > 0$ and $\rho > 0$ such that U and V satisfy Condition 6.3.1.*

Proof. Since Γ is compact and Lipschitz, there exists a finite cover of Γ consisting of open balls such that Γ is the graph of a Lipschitz function in each one. There exists $\lambda > 0$ that bounds the Lipschitz constants of these functions, and there exists $k > 0$ such that if $\boldsymbol{x}, \boldsymbol{y} \in \Gamma$ satisfy $|\boldsymbol{x} - \boldsymbol{y}| < k$ then there is a ball in the cover containing both $\boldsymbol{x}$ and $\boldsymbol{y}$. Let $\boldsymbol{u} \in U$ and $\boldsymbol{v} \in V$ such that $|\boldsymbol{u} - \boldsymbol{v}| < k$. Denote by B a ball in the cover that contains them both, and denote by φ the function such that Γ is the graph of φ in B. By rotation we may take $\varphi : \mathbb{R}^{m-1} \to \mathbb{R}$, with all $\boldsymbol{z} \in B$ satisfying

$$\boldsymbol{z} \in \Gamma \quad \Longleftrightarrow \quad z_m = \varphi(\boldsymbol{z}'),$$

where we have written $\boldsymbol{z} = (\boldsymbol{z}', z_m)$ with $\boldsymbol{z}' \in \mathbb{R}^{m-1}$.

Consider the closed line segment in $\mathbb{R}^{m-1}$ connecting $\boldsymbol{u}'$ and $\boldsymbol{v}'$. Since $\boldsymbol{u} \in U$, $\boldsymbol{v} \in V$, and U and V are closed, we find that there exists $\boldsymbol{w}'$ on the line segment such that $\boldsymbol{w} := (\boldsymbol{w}', \varphi(\boldsymbol{w}')) \in U \cap V$. The fact that $\boldsymbol{w} \in U \cap V$ implies that $\operatorname{dist}(\boldsymbol{z}, U \cap V) \leqslant |\boldsymbol{z} - \boldsymbol{w}|$ for each $\boldsymbol{z} \in \mathbb{R}^m$, so

$$\begin{aligned}
\operatorname{dist}(\boldsymbol{u}, U \cap V) + \operatorname{dist}(\boldsymbol{v}, U \cap V) &\leqslant |\boldsymbol{u} - \boldsymbol{w}| + |\boldsymbol{v} - \boldsymbol{w}| \\
&\leqslant |\boldsymbol{u}' - \boldsymbol{w}'| + |\varphi(\boldsymbol{u}') - \varphi(\boldsymbol{w}')| + |\boldsymbol{v}' - \boldsymbol{w}'| + |\varphi(\boldsymbol{v}') - \varphi(\boldsymbol{w}')| \\
&\leqslant (1 + \lambda)\big(|\boldsymbol{u}' - \boldsymbol{w}'| + |\boldsymbol{v}' - \boldsymbol{w}'|\big).
\end{aligned}$$

But the fact that $\boldsymbol{w}'$ is on the line segment implies that $|\boldsymbol{u}'-\boldsymbol{v}'| = |\boldsymbol{u}'-\boldsymbol{w}'| + |\boldsymbol{w}'-\boldsymbol{v}'|$, so

$$\operatorname{dist}(\boldsymbol{u}, U\cap V) + \operatorname{dist}(\boldsymbol{v}, U\cap V) \leqslant (1+\lambda)|\boldsymbol{u}'-\boldsymbol{v}'| \leqslant (1+\lambda)|\boldsymbol{u}-\boldsymbol{v}|.$$

The result therefore holds with $\rho = 1+\lambda$. □

The condition $|\boldsymbol{u}-\boldsymbol{v}| < k$ in the conclusion of the above lemma is present because the concept of having (or not having) cusps is entirely local. However, since we are only interested in compact sets we may drop this part of the condition, which will simplify calculations slightly.

Lemma 6.3.3. *Let $U, V \subseteq \mathbb{R}^m$ be compact sets such that $U\cap V$ is non-empty. Then Condition 6.3.1 holds with finite k if and only if it holds with $k=\infty$ (but not necessarily with the same ρ).*

Proof. The "if" statement is trivial (for example, choose $k = 1$) so we focus on the "only if" statement. Since U and V are bounded and $U\cap V$ is non-empty, the quantity

$$\operatorname{dist}(\boldsymbol{u}, U\cap V) + \operatorname{dist}(\boldsymbol{v}, U\cap V)$$

is bounded; denote a bound for it by R. For $|\boldsymbol{u}-\boldsymbol{v}| \geqslant k$ we have

$$\operatorname{dist}(\boldsymbol{u}, U\cap V) + \operatorname{dist}(\boldsymbol{v}, U\cap V) \leqslant R \leqslant \frac{R}{k}|\boldsymbol{u}-\boldsymbol{v}|.$$

The condition therefore holds with $k' = \infty$ and $\rho' = \max\{\rho, R/k\}$. □

We now prove a lemma that reflects the second notion of "no cusp" described at the start of this section. The proof is essentially the idea that was expressed intuitively there.

Lemma 6.3.4. *Let $U, V \subseteq \mathbb{R}^m$ satisfy Condition 6.3.1 with $k=\infty$. Then for all $\boldsymbol{z} \in \mathbb{R}^m$ we have*

$$\operatorname{dist}(\boldsymbol{z}, U\cap V) \leqslant (1+\rho)\max\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\}.$$

Proof. Let $\boldsymbol{z} \in \mathbb{R}^m$. Since U and V are closed,

$$\exists \boldsymbol{u} \in U \text{ s.t. } |\boldsymbol{z}-\boldsymbol{u}| = \operatorname{dist}(\boldsymbol{z}, U) \quad \text{and} \quad \exists \boldsymbol{v} \in V \text{ s.t. } |\boldsymbol{z}-\boldsymbol{v}| \leqslant \operatorname{dist}(\boldsymbol{z}, V).$$

We also have

$$\operatorname{dist}(\boldsymbol{z}, U\cap V) \leqslant |\boldsymbol{z}-\boldsymbol{u}| + \operatorname{dist}(\boldsymbol{u}, U\cap V), \qquad \operatorname{dist}(\boldsymbol{z}, U\cap V) \leqslant |\boldsymbol{z}-\boldsymbol{v}| + \operatorname{dist}(\boldsymbol{v}, U\cap V).$$

Summing these two inequalities and halving we obtain

$$\begin{aligned}
\operatorname{dist}(\boldsymbol{z}, U\cap V) &\leqslant \tfrac{1}{2}\big(\operatorname{dist}(\boldsymbol{z}, U) + \operatorname{dist}(\boldsymbol{z}, V)\big) + \tfrac{1}{2}\big(\operatorname{dist}(\boldsymbol{u}, U\cap V) + \operatorname{dist}(\boldsymbol{v}, U\cap V)\big) \\
&\leqslant \max\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\} + \tfrac{1}{2}\rho|\boldsymbol{u}-\boldsymbol{v}| \\
&\leqslant \max\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\} + \tfrac{1}{2}\rho\big(|\boldsymbol{z}-\boldsymbol{u}| + |\boldsymbol{z}-\boldsymbol{v}|\big) \\
&= \max\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\} + \tfrac{1}{2}\rho\big(\operatorname{dist}(\boldsymbol{z}, U) + \operatorname{dist}(\boldsymbol{z}, V)\big) \\
&\leqslant (1+\rho)\max\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\}.
\end{aligned}$$

□

Lemma 6.3.4 is, in essence, the fact that we need about Lipschitz domains. However, to apply it in practice we will need to write it out in terms of the pieces Γ_i, which is done in the next lemma. The observation that C_Ω does not depend on rescaling of Ω is a reflection of the fact that C_Ω depends only on the angles between the pieces.

Lemma 6.3.5. *Let $\Omega \subseteq \mathbb{R}^m$ satisfy Condition 5.2.7. Then there exists $C_\Omega > 0$ such that, for each distinct $i, j \in I$ and each $\boldsymbol{z} \in \mathbb{R}^m$, we have*

$$\max\big\{\operatorname{dist}(\boldsymbol{z}, \Gamma_i), \operatorname{dist}(\boldsymbol{z}, \Gamma_j)\big\} \geqslant C_\Omega \operatorname{dist}(\boldsymbol{z}, \partial^2\Omega).$$

For each $r > 0$ the scaled set $r\Omega$ satisfies the inequality with the same constant.

Proof. The result is trivial when $|I| = 1$, so assume that $|I| > 1$. Set $U = \Gamma_i$ and $V = \bigcup_{k\neq i} \Gamma_k$. We have

$$\max\big\{\operatorname{dist}(\boldsymbol{z}, \Gamma_i), \operatorname{dist}(\boldsymbol{z}, \Gamma_j)\big\} \geqslant \max\big\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\big\}.$$

Applying Lemma 6.3.2, Lemma 6.3.3 and Lemma 6.3.4, using the fact that $U \cap V \neq \emptyset$ because Ω is connected, and setting $C_\Omega := 1/(1+\rho)$, we have

$$\max\big\{\operatorname{dist}(\boldsymbol{z}, U), \operatorname{dist}(\boldsymbol{z}, V)\big\} \geqslant C_\Omega \operatorname{dist}(\boldsymbol{z}, U \cap V).$$

But, using $\Gamma_i^{(\mathrm{i})} \cap \Gamma_k^{(\mathrm{i})} = \emptyset$, we have

$$\begin{aligned} U \cap V = \Gamma_i \cap \bigcup_{k\neq i} \Gamma_k &= \Big(\Gamma_i \cap \bigcup_{k\neq i} \Gamma_k^{(\mathrm{i})}\Big) \cup \Big(\Gamma_i \cap \bigcup_{k\neq i} \Gamma_k \setminus \Gamma_k^{(\mathrm{i})}\Big) \\ &= \Big(\Gamma_i \setminus \Gamma_i^{(\mathrm{i})} \cap \bigcup_{k\neq i} \Gamma_k^{(\mathrm{i})}\Big) \cup \Big(\Gamma_i \cap \bigcup_{k\neq i} \Gamma_k \setminus \Gamma_k^{(\mathrm{i})}\Big) \\ &\subseteq \bigcup_{k\in I} \Gamma_k \setminus \Gamma_k^{(\mathrm{i})} = \partial^2\Omega, \end{aligned}$$

so

$$C_\Omega \operatorname{dist}(\boldsymbol{z}, U \cap V) \geqslant C_\Omega \operatorname{dist}(\boldsymbol{z}, \partial^2\Omega). \qquad \square$$

6.4 Composition for non-smooth boundary

In this section we prove Lemma 6.4.1, which as described at the start of this chapter is the first step in proving Theorem 5.2.8.

Lemma 6.4.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ with $\int W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, let Σ satisfy Condition 5.2.7 with $m = 2d$, let $b \in C^2(\Sigma)$, and let W, b, f satisfy Condition 5.2.3. Then there exists R such that*

$$\Big\|f\big(\operatorname{op}[W*(b\chi_\Sigma)]\big) - \operatorname{op}\big[f(W*(b\chi_\Sigma))\big]\Big\|_1 \leqslant R(b, \Sigma; W, f),$$

where, for all sufficiently large r, R satisfies the scaling property

$$R(b, \Sigma; W, f) = r^{2d-2} R(a, \Omega; W, f), \qquad \text{for } b = a(\cdot/r),\ \Sigma = r\Omega.$$

Proof. Summary. The overall structure of the proof is the same as for Lemma 6.1.1. We begin by applying Lemma 3.4.3, but this time we need $G = 2d+3$ (rather than $G = 2d+2$), and $D = G+4d+2$ as before. It suffices to bound $\mathsf{M}^{G,D}(F_1)$, and we expand the differential operator in this expression as before. The terms involving $h_{1,j}$ or $h_{2,j}$ may be bounded precisely as before. It therefore remains to bound

$$\mathsf{M}^{G,D}(g_{1,j}(\boldsymbol{x})g_{2,j}(\boldsymbol{y})-g_{2,j}(\boldsymbol{x})g_{1,j}(\boldsymbol{y})),$$

where, again,

$$g_{1,j}(\boldsymbol{z}) := \int_{\partial\Sigma} W(\boldsymbol{z}-\boldsymbol{z}')b(\boldsymbol{z}')(\boldsymbol{n}_1)_j(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}',$$

and $g_{2,j}$ is defined similarly. We may write the integral over $\partial\Sigma$ as an integral over its component pieces, giving

$$g_{1,j}(\boldsymbol{z}) = \sum_{i\in I}\int_{\Gamma_i} W(\boldsymbol{z}-\boldsymbol{z}')b(\boldsymbol{z}')(\boldsymbol{n}_1)_j(\boldsymbol{z}')\,\mathrm{d}\boldsymbol{z}' =: \sum_{i\in I} g_{1,j}^{(i)}(\boldsymbol{z}),$$

and similarly for $g_{2,j}$, so that

$$\begin{aligned}&\mathsf{M}^{G,D}(g_{1,j}(\boldsymbol{x})g_{2,j}(\boldsymbol{y})-g_{2,j}(\boldsymbol{x})g_{1,j}(\boldsymbol{y}))\\ &\quad= \sum_{i\in I}\mathsf{M}^{G,D}(g_{1,j}^{(i)}(\boldsymbol{x})g_{2,j}^{(i)}(\boldsymbol{y})-g_{2,j}^{(i)}(\boldsymbol{x})g_{1,j}^{(i)}(\boldsymbol{y})) + \sum_{\substack{i,k\in I\\ i\neq k}}\mathsf{M}_j^{(i,k)},\end{aligned}$$

where

$$\mathsf{M}_j^{(i,k)} := \mathsf{M}^{G,D}(g_{1,j}^{(i)}(\boldsymbol{x})g_{2,j}^{(k)}(\boldsymbol{y})) + \mathsf{M}^{G,D}(g_{2,j}^{(i)}(\boldsymbol{x})g_{1,j}^{(k)}(\boldsymbol{y})).$$

The collection of terms in the first summation may be bounded in the same way as in the proof of Lemma 6.1.1. The terms $\mathsf{M}_j^{(i,k)}$ represent the contribution from the "corners" $\partial^2\Omega$, and will be bounded separately. Bounding the components of the normal vector by 1, we see that they satisfy

$$\mathsf{M}_j^{(i,k)} \leqslant 2\sum_{|\boldsymbol{l}|+|\boldsymbol{m}|\leqslant D}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}}\frac{1}{\langle\boldsymbol{v}\rangle^G} f_{\boldsymbol{l},\boldsymbol{m}}(\boldsymbol{z}-\tfrac{1}{2}\boldsymbol{v},\boldsymbol{z}+\tfrac{1}{2}\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{z},$$

where

$$f_{\boldsymbol{l},\boldsymbol{m}}(\boldsymbol{x},\boldsymbol{y}) = \int_{\Gamma_i}\left|\partial^{\boldsymbol{l}} W(\boldsymbol{x}-\boldsymbol{x}')b(\boldsymbol{x}')\right|\mu_{2d-1}(\mathrm{d}\boldsymbol{x}')\int_{\Gamma_k}\left|\partial^{\boldsymbol{m}} W(\boldsymbol{y}-\boldsymbol{y}')b(\boldsymbol{y}')\right|\mu_{2d-1}(\mathrm{d}\boldsymbol{y}').$$

Notation for corners. We will denote the C^2 extensible pieces that make up $\partial^2\Sigma$ by Λ_p, where $p\in P$ and P is a finite indexing set. We choose a sufficiently small $s>0$ that Theorem 4.5.7 holds with $\tau = 2s$ (i.e. $\mathrm{tub}_{2s}(\mathrm{ext}_{2s}(\Lambda_p))$ is a tubular neighbourhood) and such that the conclusion of Lemma 4.5.8 holds (in particular, $B_s(\Lambda_p)\subseteq \mathrm{tub}_s(\mathrm{ext}_{2s}(\Lambda_p))$) for every $p\in P$. This choice may be made so that s is proportional to r as r varies. Since the result is only claimed to hold for sufficiently large r, we may assume that r is sufficiently large that $s > 2/C_\Sigma$, where C_Σ is the constant in the conclusion of Lemma 6.3.5.

Restriction of support. In order to apply tubular theory to the Γ_i, we will need to restrict the support of both $\partial^{\boldsymbol{l}} W$ and $\partial^{\boldsymbol{k}} W$ to compact regions, and also truncate the range of integration of the $\mathrm{d}\boldsymbol{v}$ integral to a compact region.

First we restrict support of $\partial^{\boldsymbol{l}} W$ in one term of $\mathsf{M}_j^{(i,k)}$. The error in replacing $\partial^{\boldsymbol{l}} W$ by $\chi_B \partial^{\boldsymbol{l}} W$, where B is the ball about $\mathbf{0}$ of radius $\frac{1}{2} C_\Sigma s - 1$, is bounded by

$$\int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \frac{1}{\langle \boldsymbol{v} \rangle^G} \Big(\tilde{f}_{\boldsymbol{l},\boldsymbol{m}}(\boldsymbol{z}-\boldsymbol{v},\boldsymbol{z}) - f_{\boldsymbol{l},\boldsymbol{m}}(\boldsymbol{z}-\boldsymbol{v},\boldsymbol{z}) \Big) \mathrm{d}\boldsymbol{v}\, \mathrm{d}\boldsymbol{z},$$

where $\tilde{f}_{\boldsymbol{l},\boldsymbol{m}}$ is defined as $f_{\boldsymbol{l},\boldsymbol{m}}$ but with $\partial^{\boldsymbol{l}} W$ replaced by $\chi_B \partial^{\boldsymbol{l}} W$. Now note that

$$\int_{\mathbb{R}^{2d}} \int_{\Gamma_i} \Big| \chi_{B^{\mathrm{c}}}(\boldsymbol{z}-\boldsymbol{x}') \partial^{\boldsymbol{l}} W(\boldsymbol{z}-\boldsymbol{x}') b(\boldsymbol{x}') \Big| \mu_{2d-1}(\mathrm{d}\boldsymbol{x}') \mathrm{d}\boldsymbol{z} = \|b\|_{L^1(\Gamma_i)} \int_{B^{\mathrm{c}}} |\partial^{\boldsymbol{l}} W(\boldsymbol{z})| \mathrm{d}\boldsymbol{z},$$

and bound

$$\int_{\Gamma_k} \Big| \partial^{\boldsymbol{m}} W(\boldsymbol{z}+\boldsymbol{v}-\boldsymbol{y}') b(\boldsymbol{y}') \Big| \mu_{2d-1}(\mathrm{d}\boldsymbol{y}') \leqslant \|b\|_{L^\infty(\Gamma_k)} \psi_{\partial^{\boldsymbol{m}} W}(0),$$

where $\psi_{\partial^{\boldsymbol{m}} W}$ is as in Lemma 4.6.6. This implies that the above integral of $\tilde{f}_{\boldsymbol{l},\boldsymbol{m}} - f_{\boldsymbol{l},\boldsymbol{m}}$ is bounded by

$$\Big(\int_{\mathbb{R}^{2d}} \frac{1}{\langle \boldsymbol{v} \rangle^G} \mathrm{d}\boldsymbol{v} \Big) \|b\|_{L^1(\Gamma_i)} \Big(\int_{B^{\mathrm{c}}} |\partial^{\boldsymbol{l}} W(\boldsymbol{z})| \mathrm{d}\boldsymbol{z} \Big) \|b\|_{L^\infty(\Gamma_k)} \psi_{\partial^{\boldsymbol{m}} W}(0).$$

But $W \in \mathscr{S}(\mathbb{R}^{2d})$ so the $\mathrm{d}\boldsymbol{z}$ integral may be bounded by a constant multiple of $1/r^k$ as $r \to \infty$ for every $k \in \mathbb{N}_0$. Choosing $k = 2$ shows that we may restrict the support of $\partial^{\boldsymbol{l}} W$ with only $O(r^{2d-2})$ error. We may restrict the support of $\partial^{\boldsymbol{k}} W$ in precisely the same way. From now on, we will use $\tilde{f}_{\boldsymbol{l},\boldsymbol{m}}$ in place of $f_{\boldsymbol{l},\boldsymbol{m}}$ without further comment.

Next we restrict the range of integration of the $\mathrm{d}\boldsymbol{v}$ integral to $|\boldsymbol{v}| \leqslant C_\Sigma s$, for which we will proceed in a similar way. We bound

$$\int_{\mathbb{R}^{2d}} \int_{\Gamma_i} \Big| \partial^{\boldsymbol{l}} W(\boldsymbol{z}-\boldsymbol{x}') b(\boldsymbol{x}') \Big| \mu_{2d-1}(\mathrm{d}\boldsymbol{x}') \mathrm{d}\boldsymbol{z} = \|b\|_{L^1(\Gamma_i)} \int_{\mathbb{R}^m} |\partial^{\boldsymbol{l}} W(\boldsymbol{z})| \mathrm{d}\boldsymbol{z},$$

$$\int_{\Gamma_k} \Big| \partial^{\boldsymbol{m}} W(\boldsymbol{z}+\boldsymbol{v}-\boldsymbol{y}') b(\boldsymbol{y}') \Big| \mu_{2d-1}(\mathrm{d}\boldsymbol{y}') \leqslant \|b\|_{L^\infty(\Gamma_k)} \psi_{\partial^{\boldsymbol{m}} W}(0),$$

so the error in restricting $|\boldsymbol{v}| \leqslant C_\Sigma s$ is bounded by a constant multiple of

$$\Big(\int_{|\boldsymbol{v}| > C_\Sigma s} \frac{1}{\langle \boldsymbol{v} \rangle^G} \mathrm{d}\boldsymbol{v} \Big) \|b\|_{L^1(\Gamma_i)} \Big(\int_{\mathbb{R}^m} |\partial^{\boldsymbol{l}} W(\boldsymbol{z})| \mathrm{d}\boldsymbol{z} \Big) \|b\|_{L^\infty(\Gamma_k)} \psi_{\partial^{\boldsymbol{m}} W}(0).$$

We may bound the $\mathrm{d}\boldsymbol{v}$ integrand by $1/\big(\langle \boldsymbol{v} \rangle^{G-1} \langle C_\Sigma s \rangle\big)$. The integral of $1/\langle \boldsymbol{v} \rangle^{G-1}$ over $\mathbb{R}^{2d}$ exists and is constant, while $1/\langle C_\Sigma s \rangle = O(1/r)$, so the overall expression is $O(r^{2d-2})$.

Corner terms. To bound $f_{\boldsymbol{l},\boldsymbol{m}}$ we apply Lemma 4.6.6 and take the maximum over all relevant $\boldsymbol{l},\boldsymbol{m}$ to obtain a single ψ; in particular, $\operatorname{supp}\psi \subseteq \big[0,\frac{1}{2}C_\Sigma s\big]$. This implies that

$$\begin{aligned}
f_{\boldsymbol{l},\boldsymbol{m}}(\boldsymbol{x},\boldsymbol{y}) &\leqslant \|b\|_{L^\infty}^2 \int_{\Gamma_i} \big|\partial^{\boldsymbol{l}} W(\boldsymbol{x}-\boldsymbol{x}')\big|\mu_{2d-1}(\mathrm{d}\boldsymbol{x}') \int_{\Gamma_k} \big|\partial^{\boldsymbol{m}} W(\boldsymbol{y}-\boldsymbol{y}')\big|\mu_{2d-1}(\mathrm{d}\boldsymbol{y}') \\
&\leqslant \|b\|_{L^\infty}^2 \psi(\operatorname{dist}(\boldsymbol{x},\Gamma_i))\psi(\operatorname{dist}(\boldsymbol{y},\Gamma_k)) \\
&\leqslant \|b\|_{L^\infty}^2 \psi(0)\psi\big(\max\{\operatorname{dist}(\boldsymbol{x},\Gamma_i),\operatorname{dist}(\boldsymbol{y},\Gamma_k)\}\big).
\end{aligned}$$

But using the general fact that $\operatorname{dist}(\boldsymbol{a}+\boldsymbol{b},\Gamma) \leqslant \operatorname{dist}(\boldsymbol{a},\Gamma)+|\boldsymbol{b}|$, we have

$$\operatorname{dist}(\boldsymbol{z},\Gamma_i) \leqslant \operatorname{dist}\big(\boldsymbol{z}+\tfrac{1}{2}\boldsymbol{v},\Gamma_i\big)+\tfrac{1}{2}|\boldsymbol{v}|, \qquad \operatorname{dist}(\boldsymbol{z},\Gamma_k) \leqslant \operatorname{dist}\big(\boldsymbol{z}-\tfrac{1}{2}\boldsymbol{v},\Gamma_k\big)+\tfrac{1}{2}|\boldsymbol{v}|.$$

Thus, using Lemma 6.3.5 and the fact that ψ is a non-increasing function, we have

$$\begin{aligned}
f_{\boldsymbol{l},\boldsymbol{m}}\big(\boldsymbol{z}+\tfrac{1}{2}\boldsymbol{v},\boldsymbol{z}-\tfrac{1}{2}\boldsymbol{v}\big) &\leqslant \|b\|_{L^\infty}^2 \psi(0)\psi\Big(\max\big\{\operatorname{dist}\big(\boldsymbol{z}+\tfrac{1}{2}\boldsymbol{v},\Gamma_i\big),\operatorname{dist}\big(\boldsymbol{z}-\tfrac{1}{2}\boldsymbol{v},\Gamma_k\big)\big\}\Big) \\
&\leqslant \|b\|_{L^\infty}^2 \psi(0)\psi\Big(\max\big\{\operatorname{dist}(\boldsymbol{z},\Gamma_i),\operatorname{dist}(\boldsymbol{z},\Gamma_k)\big\}-\tfrac{1}{2}|\boldsymbol{v}|\Big) \\
&\leqslant \|b\|_{L^\infty}^2 \psi(0)\psi\big(C_\Sigma \operatorname{dist}(\boldsymbol{z},\partial^2\Sigma)-\tfrac{1}{2}|\boldsymbol{v}|\big),
\end{aligned}$$

where for negative t we just define $\psi(t) := \psi(0)$.

Substituting this bound for $f_{\boldsymbol{l},\boldsymbol{m}}$ into the bound for $\mathsf{M}_j^{(i,k)}$ we obtain

$$\begin{aligned}
\mathsf{M}_j^{(i,k)} &\leqslant 2\|b\|_{L^\infty}^2 \psi(0) \int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{1}{\langle\boldsymbol{v}\rangle^G}\psi\big(C_\Sigma \operatorname{dist}(\boldsymbol{z},\partial^2\Sigma)-\tfrac{1}{2}|\boldsymbol{v}|\big)\mathrm{d}\boldsymbol{z}\,\mathrm{d}\boldsymbol{v} \\
&\leqslant 2\|b\|_{L^\infty}^2 \psi(0) \sum_{p\in P}\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \frac{1}{\langle\boldsymbol{v}\rangle^G}\psi\big(C_\Sigma \operatorname{dist}(\boldsymbol{z},\Lambda_p)-\tfrac{1}{2}|\boldsymbol{v}|\big)\mathrm{d}\boldsymbol{z}\,\mathrm{d}\boldsymbol{v}
\end{aligned}$$

Set $\widetilde{\psi}(\lambda) := \psi\big(C_\Sigma\lambda-\frac{1}{2}|\boldsymbol{v}|\big)$ for $\lambda \geqslant 0$. Because $-\frac{1}{2}|\boldsymbol{v}| \geqslant -\frac{1}{2}C_\Sigma s$, it follows that when $\lambda > s$ we have $C_\Sigma\lambda-\frac{1}{2}|\boldsymbol{v}| > \frac{1}{2}C_\Sigma s$; but $\psi(t)=0$ when $t > \frac{1}{2}C_\Sigma s$, so $\widetilde{\psi}(\lambda)=0$ when $\lambda > s$ i.e. $\operatorname{supp}\widetilde{\psi} \subseteq [0,s]$. We may therefore apply Lemma 4.6.7 to $\widetilde{\psi}$, giving

$$\mathsf{M}_j^{(i,k)} \lesssim \|b\|_{L^\infty}^2 \sum_{p\in P}\mu_{2d-2}(\operatorname{ext}_{2s}(\Lambda_p)) \int_{\mathbb{R}^{2d}}\int_0^s \frac{1}{\langle\boldsymbol{v}\rangle^G}\lambda\psi\big(C_\Sigma\lambda-\tfrac{1}{2}|\boldsymbol{v}|\big)\mathrm{d}\lambda\,\mathrm{d}\boldsymbol{v}.$$

Certainly $\sum_{p\in P}\mu_{2d-2}(\operatorname{ext}_{2s}(\Lambda_p)) \propto r^{2d-2}$, so it remains to show that the $\mathrm{d}\lambda\,\mathrm{d}\boldsymbol{v}$ integral is bounded by a constant. Changing variables $\lambda' := C_\Sigma\lambda-\frac{1}{2}|\boldsymbol{v}|$, then extending the range of integration of $\mathrm{d}\lambda'$ to $+\infty$ and breaking it into the negative and positive parts, we find that the above integral equals

$$\begin{aligned}
&\frac{1}{C_\Sigma^2}\int_{\mathbb{R}^{2d}}\int_{-|\boldsymbol{v}|/2}^{C_\Sigma s-|\boldsymbol{v}|/2} \frac{1}{\langle\boldsymbol{v}\rangle^G}\big(\lambda'+\tfrac{1}{2}|\boldsymbol{v}|\big)\psi(\lambda')\mathrm{d}\lambda'\,\mathrm{d}\boldsymbol{v} \\
&\quad\leqslant \frac{1}{C_\Sigma^2}\int_{\mathbb{R}^{2d}}\int_{-|\boldsymbol{v}|/2}^{0} \frac{|\boldsymbol{v}|}{\langle\boldsymbol{v}\rangle^G}\psi(0)\mathrm{d}\lambda'\,\mathrm{d}\boldsymbol{v} + \frac{1}{C_\Sigma^2}\int_{\mathbb{R}^{2d}}\int_0^\infty \frac{\langle\boldsymbol{v}\rangle}{\langle\boldsymbol{v}\rangle^G}\langle\lambda'\rangle\psi(\lambda')\mathrm{d}\lambda'\,\mathrm{d}\boldsymbol{v} \\
&\quad= \frac{1}{2C_\Sigma^2}\bigg(\int_{\mathbb{R}^{2d}}\frac{|\boldsymbol{v}|^2}{\langle\boldsymbol{v}\rangle^G}\mathrm{d}\boldsymbol{v}\bigg)\psi(0) + \frac{1}{C_\Sigma^2}\bigg(\int_{\mathbb{R}^{2d}}\frac{1}{\langle\boldsymbol{v}\rangle^{G-1}}\mathrm{d}\boldsymbol{v}\bigg)\bigg(\int_0^\infty\langle\lambda'\rangle\psi(\lambda')\mathrm{d}\lambda'\bigg).
\end{aligned}$$

A conclusion of Lemma 6.3.5 is that C_Σ does not depend on rescaling, and a conclusion of Lemma 4.6.6 is that ψ does not depend on Σ at all, so this bound is independent of r. ☐

6.5 Trace asymptotics for non-smooth boundary

In this section we prove Lemma 6.5.1, which is the second step in proving the Szegő theorem for piecewise C^2 boundary, as discussed at the start of this chapter. To prove it we will break $\partial\Omega$ into its component pieces, and then each piece may be treated as the smooth boundary was in §6.2.

Lemma 6.5.1. *Let $W \in \mathscr{S}(\mathbb{R}^{2d})$ with $\int W(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} = 1$, let Σ satisfy Condition 5.2.7 with $m = 2d$, let $b \in C^2(\Sigma)$, and let W, b, f satisfy Condition 5.2.3. Then there exists R such that, using Notation 3.4.1, we have*

$$\left|\int_{\mathbb{R}^{2d}} f(W*(b\chi_\Sigma)(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{z} - \Big(A_0(b,\Sigma,f) + A_1(b,\Sigma,f;W)\Big)\right| \leqslant R(b,\Sigma;W,f),$$

where R satisfies the scaling property

$$R(b,\Sigma;W,f) = r^{2d-2}R(a,\Omega;W,f), \qquad \text{for } b = a(\cdot/r),\ \Sigma = r\Omega.$$

Proof. Summary. Just as in Lemma 6.2.1, set

$$\begin{aligned} I_1 &:= \int_{\mathbb{R}^{2d}} \Big(f(W*(\chi_\Sigma b)(\boldsymbol{z})) - W*(\chi_\Sigma f(b))(\boldsymbol{z})\Big)\,\mathrm{d}\boldsymbol{z}, \\ I_5 &:= \int_{\partial\Sigma}\int_{\mathbb{R}} \Big(f(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)b(\boldsymbol{u})) - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)f(b(\boldsymbol{u}))\Big)\,\mathrm{d}\lambda\,\mu_{2d-1}(\mathrm{d}\boldsymbol{u}). \end{aligned}$$

We must again show that when $b = a(\cdot/r)$ and $\Sigma = r\Omega$, we have $I_1 = I_5 + O(r^{2d-2})$. To do this, we will begin by noticing that it suffices to consider f and W that are compactly supported. We will then approximate I_1 with a similar integral I_2 in the same way as before. However, at that point we decompose I_2 into a sum corresponding to the decomposition of $\partial\Sigma$ into the pieces Γ_i. We then show that each of these may approximated by I_5 for each piece in precisely the same way as in Lemma 6.2.1. The final result follows because for any $h \in L^1(\partial\Sigma)$ we have

$$\int_{\partial\Sigma} h(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = \sum_{i\in I}\int_{\Gamma_i} h(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}.$$

Step 1: Restrict support of f. Precisely as before, the integrals depend on f only for values in a fixed compact region, so we may restrict f to a compact set with zero error.

Step 2: Restrict support of W. This also works in precisely the same way as before. The only difference is that this time we choose the support to be in the ball $B_{s/2}(\mathbf{0})$, where $s > 0$ is sufficiently small that the conditions of Lemma 4.5.11 hold (so the conclusions of the preceding lemmas in that section hold) for every piece Γ_i of the boundary $\partial\Sigma$ and that the conclusions of Theorem 4.5.7 (with $2s \leqslant \tau$) and Lemma 4.5.8 hold for every piece of $\partial^2\Sigma$. As before, $s \propto r$, so the error in restricting W to this ball is asymptotically very small.

Step 3: Extract b from convolution. We again set

$$I_2 := \int_{\mathbb{R}^{2d}} \Big(f(W * \chi_\Sigma(\boldsymbol{z}) b(\boldsymbol{z})) - W * \chi_\Sigma(\boldsymbol{z}) f(b(\boldsymbol{z})) \Big) \mathrm{d}\boldsymbol{z}.$$

We may bound $|I_2 - I_3|$ as we did in the smooth boundary case, and most of the resulting terms make no use of the geometry of $\partial\Sigma$ so may be bounded in the same way as there. The exception is in bounding

$$\|f''\|_{L^\infty} \|b\|_{L^\infty(\mathbb{R}^{2d})} \int_{\mathbb{R}^{2d}} |V * \chi_\Sigma(\boldsymbol{z}) V * \chi_{\Sigma^c}(\boldsymbol{z}) \nabla b(\boldsymbol{z})| \,\mathrm{d}\boldsymbol{z}.$$

We may still use Lemma 4.6.5, so this is bounded by

$$\begin{aligned} &\|f''\|_{L^\infty} \|b\|_{L^\infty(\mathbb{R}^{2d})} \|\nabla b\|_{L^\infty(\mathbb{R}^{2d})} \int_{\mathbb{R}^{2d}} \psi_V(\mathrm{dist}(\boldsymbol{z}, \partial\Sigma)) \,\mathrm{d}\boldsymbol{z} \\ &\leqslant \|f''\|_{L^\infty} \|b\|_{L^\infty(\mathbb{R}^{2d})} \|\nabla b\|_{L^\infty(\mathbb{R}^{2d})} \sum_{i \in I} \int_{\mathbb{R}^{2d}} \psi_V(\mathrm{dist}(\boldsymbol{z}, \Gamma_i)) \,\mathrm{d}\boldsymbol{z}, \end{aligned}$$

where $\operatorname{supp}\psi_V \subseteq \left[0, \frac{1}{2}s\right]$. We may therefore apply Lemma 4.6.7 to show that the integral is $O(r^{2d-1})$, and so the overall bound is $O(r^{2d-2})$.

Reduction to C^2 pieces: summary. We define the analogue of the integral I_2 for each piece Γ_i of the boundary $\partial\Sigma$ as follows. Define Λ_i and Σ_i for each $i \in I$ as in Lemma 4.5.11 (so Σ_i is a half-tube about $\mathrm{ext}_{2s}(\Gamma_i)$, and Λ_i is a narrower tube about $\Gamma_i^{(\mathrm{i})}$). Then

$$J_2(i) := \int_{\mathbb{R}^{2d}} \chi_{\Lambda_i}(\boldsymbol{z}) \Big(f(W * \chi_{\Sigma_i}(\boldsymbol{z}) b(\boldsymbol{z})) - W * \chi_{\Sigma_i}(\boldsymbol{z}) f(b(\boldsymbol{z})) \Big) \mathrm{d}\boldsymbol{z}.$$

We now show that $\left| I_2 - \sum_{i \in I} J_2(i) \right| = O(r^{2d-2})$; this is the main part of the proof of this lemma. For any region $A \subseteq \mathbb{R}^{2d}$ we use the notation

$$\omega_A(\boldsymbol{z}) := f(W * \chi_A(\boldsymbol{z}) b(\boldsymbol{z})) - W * \chi_A(\boldsymbol{z}) f(b(\boldsymbol{z})).$$

In particular, I_2 is the integral of ω_Σ and $J_2(i)$ is the integral of $\chi_{\Lambda_i} \omega_{\Sigma_i}$. These are supported within $B_{s/2}(\partial\Sigma)$, so it suffices to consider points in this region. For any $\boldsymbol{z} \in B_{s/2}(\partial\Sigma)$ there is a $\boldsymbol{u} \in \partial\Sigma$ such that $|\boldsymbol{z} - \boldsymbol{u}| = \mathrm{dist}(\boldsymbol{z}, \partial\Sigma)$ (not necessarily unique, but any choice will do). There are two possible cases: either $\boldsymbol{u} \in \partial^2\Sigma$ or $\boldsymbol{u} \in \Gamma_j^{(\mathrm{i})}$ for some $j \in I$. In both cases we will prove that

$$\left| \omega_\Sigma(\boldsymbol{z}) - \sum_{i \in I} \chi_{\Lambda_i}(\boldsymbol{z}) \omega_{\Sigma_i}(\boldsymbol{z}) \right| \leqslant \Big((|I|+1) \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 + \|f'\|_{L^\infty} |b(\boldsymbol{z})| \Big) \varphi(\mathrm{dist}(\boldsymbol{z}, \partial^2\Sigma)), \qquad (*)$$

where φ is a quickly decaying function that does not depend on b or Σ except through the constant C_Σ from the conclusion of Lemma 6.3.5. Integrating this over $\boldsymbol{z}$ and applying Lemma 4.6.7 shows that $\left| I_2 - \sum_{i \in I} J_2(i) \right| = O(r^{2d-2})$.

Reduction to C^2 pieces: bounds for ω_A. Before tackling the two cases described above, we will need two preliminary facts about ω_A: for any sets $A, B \subseteq \mathbb{R}^{2d}$ we have

$$|\omega_A(\boldsymbol{z})| \leqslant \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 \psi_W(\mathrm{dist}(\boldsymbol{z}, \partial A)),$$
$$|\omega_A(\boldsymbol{z}) - \omega_B(\boldsymbol{z})| \leqslant 2\|f'\|_{L^\infty} |b(\boldsymbol{z})| |W| * \chi_{A \Delta B}(\boldsymbol{z}),$$

where Δ denotes symmetric difference. When applying the first bound with $A = \Sigma_i$, we will use the fact that when $\boldsymbol{z} \in \Lambda_i$ we have $\mathrm{dist}(\boldsymbol{z}, \partial \Sigma_i) = \mathrm{dist}(\boldsymbol{z}, \Gamma_i)$ (by Lemma 4.5.11).

For the bound on $|\omega_A(\boldsymbol{z})|$, write $f(t) = t g(t)$ (see Lemma 5.1.5), so that

$$\omega_A(\boldsymbol{z}) = W * \chi_A(\boldsymbol{z}) b(\boldsymbol{z}) \Big(g(W * \chi_A(\boldsymbol{z}) b(\boldsymbol{z})) - g(b(\boldsymbol{z})) \Big),$$

so by the mean value theorem

$$\begin{aligned} |\omega_A(\boldsymbol{z})| &\leqslant \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 |1 - W * \chi_A(\boldsymbol{z})| |W * \chi_A(\boldsymbol{z})| \\ &= \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 |W * \chi_{A^c}(\boldsymbol{z})| |W * \chi_A(\boldsymbol{z})|, \end{aligned}$$

and the stated bound follows by Lemma 4.6.5.

For the bound on $|\omega_A(\boldsymbol{z}) - \omega_B(\boldsymbol{z})|$ we compare the respective two terms in ω_A, ω_B separately. For the first term, we have

$$|f(W * \chi_A(\boldsymbol{z}) b(\boldsymbol{z})) - f(W * \chi_B(\boldsymbol{z}) b(\boldsymbol{z}))| \leqslant \|f'\|_{L^\infty} |b(\boldsymbol{z})| |W * \chi_A(\boldsymbol{z}) - W * \chi_B(\boldsymbol{z})|,$$

and, for the second term, we have

$$\begin{aligned} |W * \chi_A(\boldsymbol{z}) f(b(\boldsymbol{z})) - W * \chi_B(\boldsymbol{z}) f(b(\boldsymbol{z}))| &\leqslant |f(b(\boldsymbol{z}))| |W * \chi_A(\boldsymbol{z}) - W * \chi_B(\boldsymbol{z})| \\ &\leqslant \|f'\|_{L^\infty} |b(\boldsymbol{z})| |W * \chi_A(\boldsymbol{z}) - W * \chi_B(\boldsymbol{z})|. \end{aligned}$$

Thus

$$|\omega_A(\boldsymbol{z}) - \omega_B(\boldsymbol{z})| \leqslant 2\|f'\|_{L^\infty} |b(\boldsymbol{z})| |W * \chi_A(\boldsymbol{z}) - W * \chi_B(\boldsymbol{z})|,$$

and the stated bound follows by noting that

$$|W * \chi_A(\boldsymbol{z}) - W * \chi_B(\boldsymbol{z})| = |W * (\chi_A - \chi_B)(\boldsymbol{z})| \leqslant |W| * \chi_{A \Delta B}(\boldsymbol{z}).$$

Reduction to C^2 pieces, case 1: $\boldsymbol{u} \in \partial^2 \Sigma$. We will bound the integrands in I_2 and $J_2(i)$ separately. We have $\mathrm{dist}(\boldsymbol{z}, \partial \Sigma) = \mathrm{dist}(\boldsymbol{z}, \partial^2 \Sigma)$ so

$$|\omega_\Sigma(\boldsymbol{z})| \leqslant \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 \psi_W(\mathrm{dist}(\boldsymbol{z}, \partial^2 \Sigma)).$$

For each $i \in I$ we have $\mathrm{dist}(\boldsymbol{z}, \Gamma_i) \geqslant \mathrm{dist}(\boldsymbol{z}, \partial \Sigma) = \mathrm{dist}(\boldsymbol{z}, \partial^2 \Sigma)$, so

$$|\omega_{\Sigma_i}(\boldsymbol{z})| \leqslant \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 \psi_W(\mathrm{dist}(\boldsymbol{z}, \partial^2 \Sigma)).$$

Choosing $\varphi \geqslant \psi_W$, this satisfies the bound in equation $(*)$ above.

Reduction to C^2 pieces, case 2: $\boldsymbol{u} \in \Gamma_j^{(\mathrm{i})}$ for some $j \in I$. We will bound

$$\left|\omega_\Sigma(\boldsymbol{z}) - \sum_{i\in I} \chi_{\Lambda_i}(\boldsymbol{z})\omega_{\Sigma_i}(\boldsymbol{z})\right| \leqslant |\omega_\Sigma(\boldsymbol{z}) - \omega_{\Sigma_j}(\boldsymbol{z})| + \sum_{\substack{i\in I\\ i\neq j}} \chi_{\Lambda_i}(\boldsymbol{z})|\omega_{\Sigma_i}(\boldsymbol{z})|.$$

For the second collection of terms, note that for all $i \in I$ such that $i \neq j$ we have $\operatorname{dist}(\boldsymbol{z}, \Gamma_i) \geqslant \operatorname{dist}(\boldsymbol{z}, \Gamma_j)$, so by Lemma 6.3.5 we have

$$\operatorname{dist}(\boldsymbol{z}, \Gamma_i) = \max\{\operatorname{dist}(\boldsymbol{z}, \Gamma_i), \operatorname{dist}(\boldsymbol{z}, \Gamma_j)\} \geqslant C_\Sigma \operatorname{dist}(\boldsymbol{z}, \partial^2\Sigma)$$

Using the fact that ψ_W is decreasing we obtain

$$|\omega_{\Sigma_i}(\boldsymbol{z})| \leqslant \|f''\|_{L^\infty} |b(\boldsymbol{z})|^2 \psi_W(C_\Sigma \operatorname{dist}(\boldsymbol{z}, \partial^2\Sigma)).$$

Choosing $\varphi(t) \geqslant \psi_W(C_\Sigma t)$, this satisfies the bound in $(*)$. We now bound the first term, $|\omega_\Sigma - \omega_{\Sigma_j}|$. Using the bound proved earlier we have

$$|\omega_\Sigma(\boldsymbol{z}) - \omega_{\Sigma_j}(\boldsymbol{z})| \leqslant 2\|f'\|_{L^\infty} |b(\boldsymbol{z})| \, |W| * \chi_{\Sigma\Delta\Sigma_j}(\boldsymbol{z}).$$

We now apply the final part of Lemma 4.5.11 with $V := \bigcup_{i\neq j} \Gamma_i$ and $\ell^{\boldsymbol{z}} := \min\left\{\frac{1}{2}s, \operatorname{dist}(\boldsymbol{z}, V)\right\}$, which says that

$$\Sigma_i \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z}) = \Sigma \cap B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z}),$$

so $\Sigma\Delta\Sigma_j \subseteq B_{\ell^{\boldsymbol{z}}}(\boldsymbol{z})^{\mathrm{c}}$. Setting $\gamma(\lambda) := \int_{|\boldsymbol{z}'|>\lambda} |W(\boldsymbol{z}')| \, \mathrm{d}\boldsymbol{z}'$ (so that $\gamma(\lambda) = 0$ whenever $\lambda > \frac{1}{2}s$), we thus have

$$|W| * \chi_{\Sigma\Delta\Sigma_j}(\boldsymbol{z}) \leqslant \gamma(\ell^{\boldsymbol{z}}) = \gamma(\operatorname{dist}(\boldsymbol{z}, V)) = \gamma(\min_{i\neq j} \operatorname{dist}(\boldsymbol{z}, \Gamma_i)).$$

For each $i \neq j$ we have $\operatorname{dist}(\boldsymbol{z}, \Gamma_i) \geqslant \operatorname{dist}(\boldsymbol{z}, \Gamma_j)$, so by Lemma 6.3.5 we have

$$\operatorname{dist}(\boldsymbol{z}, \Gamma_i) = \max\{\operatorname{dist}(\boldsymbol{z}, \Gamma_i), \operatorname{dist}(\boldsymbol{z}, \Gamma_j)\} \geqslant C_\Sigma \operatorname{dist}(\boldsymbol{z}, \partial^2\Sigma),$$

and since γ is decreasing we obtain

$$|\omega_\Sigma(\boldsymbol{z}) - \omega_{\Sigma_j}(\boldsymbol{z})| \leqslant 2\|f'\|_{L^\infty} |b(\boldsymbol{z})| \gamma(C_\Sigma \operatorname{dist}(\boldsymbol{z}, \partial^2\Sigma)).$$

Choosing $\varphi(t) \geqslant 2\gamma(C_\Sigma t)$, this also satisfies the bound in $(*)$.

Steps 4, 5 and 6. The remaining steps now proceed in analogy to the smooth boundary case. In step 4 we may still use Lemma 4.6.8 (this time using Lemma 4.5.10 for the normal vector field). In step 5 we use the third part of Remark 4.5.9 in place of Lemma 4.2.6. In step 6 we use Lemma 4.6.2 precisely as in the smooth case. □

6.6 Proof for cusp boundary

In this section we prove Theorem 5.6.1, which is the Szegő theorem for symbols that have a cusp boundary under some simplifying assumptions (including that $f(t) = t^2$). The proof follows the idea discussed at the end of §5.6.

Proof of Theorem 5.6.1. Summary. Overall, we proceed in the same way as the proof of the main result, which is discussed at the start of this chapter. We again begin by considering a rescaled form of the symbol: we write

$$T_r[\chi_\Omega a] = \operatorname{op}[W * (\chi_\Sigma b)], \qquad \text{where } b := a(\cdot/r),\ \Sigma := r\Omega.$$

Similarly, we define

$$\begin{aligned} \Sigma_1 &:= r\Omega_1 = \{(x,y)\in\mathbb{R}^2 : y \leqslant \sigma(x)\}, \qquad \text{where } \sigma(x) = r\omega\left(\frac{x}{r}\right), \\ \Sigma_2 &:= r\Omega_2 = \{(x,y)\in\mathbb{R}^2 : y \geqslant 0\}. \end{aligned}$$

There are again two parts to this proof: composition and trace asymptotics. However, the choice of $f(t) = t^2$ renders the composition part trivial, because for any real-valued Weyl symbol q we have

$$\operatorname{tr}\big(\operatorname{op}[q]\big)^2 = \|\operatorname{op}[q]\|_2^2 = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}} \big(q(\boldsymbol{z})\big)^2\,\mathrm{d}\boldsymbol{z},$$

where $\|\cdot\|_2$ is the Hilbert–Schmidt norm (see, for example, Birman and Solomjak, 1987, §11.3 for the first identity and Shubin, 2001, Proposition 27.1 for the second). (In this case $d = 1$, so the integral is over $\mathbb{R}^2$.) Continuing to follow the discussion at the start of the chapter, we write

$$\begin{aligned} \operatorname{tr}\big(\operatorname{op}[W*(\chi_\Sigma b)]\big)^2 &= \frac{1}{2\pi}\int_{\mathbb{R}^2}\big(W*(\chi_\Sigma b)(\boldsymbol{z})\big)^2\,\mathrm{d}\boldsymbol{z} \\ &= \underbrace{\frac{1}{2\pi}\int_{\mathbb{R}^2} W*(\chi_\Sigma b)^2(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}}_{B_0} + \underbrace{\frac{1}{2\pi}\int_{\mathbb{R}^2}\Big(\big(W*(\chi_\Sigma b)(\boldsymbol{z})\big)^2 - W*(\chi_\Sigma b)^2(\boldsymbol{z})\Big)\mathrm{d}\boldsymbol{z}}_{B_1}. \end{aligned}$$

As before, the first term B_0 equals A_0 due to the second part of Lemma 5.1.2, and the second term B_1 is noticeably similar to A_1. In steps 1 and 2 below, we will show that the second term is indeed approximately equal to A_1, with $O(1)$ error except for a specified remainder term. In steps 3 to 6, we show that this remainder is $\Theta(r\omega^{-1}(1/r))$.

Step 1: Put A_1 and B_1 in a comparable form. We wish to compare B_1 against

$$\begin{aligned} A_1(b,\Sigma,f;W) &= \frac{1}{2\pi}\int_{\partial\Sigma}\int_{\mathbb{R}}\Big(\big(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)b(\boldsymbol{u})\big)^2 - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)\big(b(\boldsymbol{u})\big)^2\Big)\mathrm{d}\lambda\,\mu_1(\mathrm{d}\boldsymbol{u}) \\ &= \frac{1}{2\pi}\int_{\partial\Sigma_1\cap H}\int_{\mathbb{R}}\Big(\big(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)b(\boldsymbol{u})\big)^2 - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)\big(b(\boldsymbol{u})\big)^2\Big)\mathrm{d}\lambda\,\mu_1(\mathrm{d}\boldsymbol{u}) \\ &\quad + \frac{1}{2\pi}\int_{\partial\Sigma_2\cap H}\int_{\mathbb{R}}\Big(\big(Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)b(\boldsymbol{u})\big)^2 - Q_{\boldsymbol{n}(\boldsymbol{u})}(\lambda)\big(b(\boldsymbol{u})\big)^2\Big)\mathrm{d}\lambda\,\mu_1(\mathrm{d}\boldsymbol{u}), \end{aligned}$$

where $H := \mathbb{R}_+ \times \mathbb{R}$ is the half space of points satisfying $x > 0$. The most immediately noticeable difference between A_1 and B_1 is that A_1 is an integral over $\partial\Sigma\times\mathbb{R}$ (concentrated near to $\partial\Sigma\times\{0\}$) while B_1 is an integral over $\mathbb{R}^2$ (concentrated near to $\partial\Sigma$). We showed in Lemma 6.2.1 (trace asymptotics for smooth boundaries) that it is straightforward to switch between these two forms and in this step we work in exactly the same way to put A_1 and B_1 in a similar form. In fact, the form of most use here is somewhere between the two extremes, so we will need to manipulate both integrals. Specifically, we will show that $A_1 = \widetilde{A}_1 + O(1)$ and $B_1 = \widetilde{B}_1 + O(1)$ where

$$\begin{aligned}\widetilde{A}_1 &:= \frac{1}{2\pi}\int_0^\infty\int_{-\infty}^\infty\Big(\big(W*\chi_{\Sigma_1}(x,y)b(x,y)\big)^2 - W*\chi_{\Sigma_1}(x,y)\big(b(x,y)\big)^2\Big)\,\mathrm{d}y\,\mathrm{d}x\\ &\quad+\frac{1}{2\pi}\int_0^\infty\int_{-\infty}^\infty\Big(\big(W*\chi_{\Sigma_2}(x,y)b(x,y)\big)^2 - W*\chi_{\Sigma_2}(x,y)\big(b(x,y)\big)^2\Big)\,\mathrm{d}y\,\mathrm{d}x,\\ \widetilde{B}_1 &:= \frac{1}{2\pi}\int_0^\infty\int_{-\infty}^\infty\Big(\big(W*\chi_{\Sigma}(x,y)b(x,y)\big)^2 - W*\chi_{\Sigma}(x,y)\big(b(x,y)\big)^2\Big)\,\mathrm{d}y\,\mathrm{d}x.\end{aligned}$$

For A_1, we apply steps 4, 5 and 6 of the proof of Lemma 6.2.1 to $\widetilde{A}_1$:

- Step 4 (approximate b by its value on $\partial\Sigma$): This step is trivial because b already equals its value on the boundary. For all $\boldsymbol{u}$ such that $u_1 \leqslant 2r-\ell$ (where ℓ is a number independent of r such that $\operatorname{supp} W \subseteq B_\ell(\mathbf{0})$) we have

  $$b(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})) = 1 = b(\boldsymbol{u}),$$

  while for $u_1 \geqslant r+\ell$ we have $\boldsymbol{n}(\boldsymbol{u}) = (0,1)$ so $b(\boldsymbol{u}+\lambda\boldsymbol{n}(\boldsymbol{u})) = b(\boldsymbol{u})$.

- Step 5 (approximate Σ locally by a half space): We again start by applying Lemma 4.3.3 (the tubular change of variables), with the restriction that $\boldsymbol{u}\in H$ in each integral translating to the restriction that $x \geqslant 0$. The rest of this step is trivial for $\boldsymbol{u}\in\partial\Sigma$ that are outside the range $-\ell < u_1 < r+\ell$ because $\partial\Sigma_1$ and $\partial\Sigma_2$ are straight there. For the remaining $\boldsymbol{u}$, working as we did in the proof of Lemma 6.2.1, we obtain the remainder bound

  $$\|f'\|_{L^\infty}(r+2\ell)\sup_{\boldsymbol{u}\in\partial\Sigma} J(\boldsymbol{u}),$$

  where we again have $J(\boldsymbol{u}) \propto 1/r$, so this remainder is $O(1)$.

- Step 6 (neglect Jacobian): This is identical to this step in the proof of Lemma 6.2.1.

For B_1, we need only apply one step of the proof of Lemma 6.2.1 to B_1:

- Step 3 (extract b from convolution): For $x < 2r$ we have $b(x,y) = 1$, so for $x < 2r-\ell$ we have

  $$\begin{gathered}\big(W*(\chi_\Sigma b)\big)^2 = \big(W*\chi_\Sigma\big)^2 = \big((W*\chi_\Sigma)\,b\big)^2,\\ W*(\chi_\Sigma b)^2 = W*(\chi_\Sigma)^2 = (W*\chi_\Sigma)\,b^2.\end{gathered}$$

For $x > 3r$ we have $b(x,y) = 0$ so the integrands are also equal for $x > 3r + \ell$. For $2r - \ell < x < 3r + \ell$, we may proceed precisely as in step 3 of the proof of Lemma 6.2.1. The only term depending on the geometry of $\partial\Sigma$ is

$$\|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^2)} \int_{2r-\ell}^{3r+\ell}\int_{-\infty}^{\infty} |V * \chi_\Sigma(x,y) V * \chi_{\Sigma^c}(x,y) \nabla b(x,y)| \,\mathrm{d}y\,\mathrm{d}x,$$

(where $V(\boldsymbol{z}') := (1+|\boldsymbol{z}'|)|W(\boldsymbol{z}')|$) and we may again apply Lemma 4.6.5 (which holds for any set) to bound this by

$$\begin{aligned}
&\|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^2)}\|\nabla b\|_{L^\infty(\mathbb{R}^2)} \int_{2r-\ell}^{3r+\ell}\int_{-\infty}^{\infty} \psi_V\Big(\operatorname{dist}\big((x,y),\partial\Sigma\big)\Big)\,\mathrm{d}y\,\mathrm{d}x \\
&\quad\leqslant \|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^2)}\|\nabla b\|_{L^\infty(\mathbb{R}^2)} \sum_{j\in\{1,2\}} \int_{2r-\ell}^{3r+\ell}\int_{-\infty}^{\infty} \psi_V\Big(\operatorname{dist}\big((x,y),\partial\Sigma_j\big)\Big)\,\mathrm{d}y\,\mathrm{d}x \\
&\quad= 2(r+2\ell)\|f''\|_{L^\infty}\|b\|_{L^\infty(\mathbb{R}^2)}\|\nabla b\|_{L^\infty(\mathbb{R}^2)} \int_{-\infty}^{\infty} \psi_V\big(|y|\big)\,\mathrm{d}y.
\end{aligned}$$

The $\mathrm{d}y$ integral is $O(1)$ while $\|\nabla b\|_{L^\infty(\mathbb{R}^2)} = O(1/r)$, so the bound is $O(1)$ overall.

<u>Step 2: Reduction to cusp.</u> For any set $\Lambda \subseteq \mathbb{R}^2$, denote $\zeta_\Lambda := W * \chi_\Lambda$; thus ζ_Λ is a smoothed out indicator function, with $\zeta_\Lambda(\boldsymbol{z}) = \chi_\Lambda(\boldsymbol{z})$ for $\operatorname{dist}(\boldsymbol{z},\partial\Lambda) > \ell$. Because of the linearity of convolution, this satisfies $1 - \zeta_\Lambda = W * (1-\chi_\Lambda) = \zeta_{\Lambda^c}$; in particular,

$$(W*\chi_\Lambda)^2 - W*\chi_\Lambda = -(W*\chi_\Lambda)(1 - W*\chi_\Lambda) = -\zeta_\Lambda\zeta_{\Lambda^c}.$$

Denote

$$R := \int_0^\infty \int_{-\infty}^{\infty} \zeta_{\Sigma_1^c}(x,y)\zeta_{\Sigma_2^c}(x,y)\,\mathrm{d}y\,\mathrm{d}x,$$

which has non-zero integrand only in the region of the cusp. In this step we will show that

$$\widetilde{B}_1 = \widetilde{A}_1 + 2R + O(1),$$

so it suffices to show that $R = \Theta(r\omega^{-1}(1/r))$ in order to prove the result.

In order to demonstrate this relationship we will compare the integrands in three separate regions of the $\mathbb{R}^2$ plane: $x < 0$, $0 \leqslant x \leqslant 2r - \ell$ and $x > 2r - \ell$ (where $\operatorname{supp} W \subseteq B_\ell(\mathbf{0})$). For $x < 0$ the integrand of $\widetilde{A}_1$ is identically 0, while the integrand of $\widetilde{B}_1$ is $-\zeta_\Sigma\zeta_{\Sigma^c}$, which by Lemma 4.6.5 satisfies

$$\begin{aligned}
\int_{-\infty}^{0}\int_{-\infty}^{\infty} \zeta_\Sigma(x,y)\zeta_{\Sigma^c}(x,y)\,\mathrm{d}y\,\mathrm{d}x &\leqslant \int_{-\infty}^{0}\int_{-\infty}^{\infty} \psi_W\Big(\operatorname{dist}\big((x,y),\partial\Sigma\big)\Big)\,\mathrm{d}y\,\mathrm{d}x \\
&\leqslant \int_{-\infty}^{0}\int_{-\infty}^{\infty} \psi_W\Big(\big|(x,y)-(0,0)\big|\Big)\,\mathrm{d}y\,\mathrm{d}x = O(1).
\end{aligned}$$

For $x \geqslant 2r - \ell$, for sufficiently large r we have $\sigma(x) = r > 2\ell$ so the integrand of $\widetilde{B}_1$ is precisely equal to the integrand of $\widetilde{A}_1$. Finally, for $0 \leqslant x \leqslant 2r - \ell$ the integrands of $\widetilde{A}_1$ and $\widetilde{B}_1$ are, respectively,

$$-\big(\zeta_{\Sigma_1}\zeta_{\Sigma_1^c} + \zeta_{\Sigma_2}\zeta_{\Sigma_2^c}\big), \qquad -\zeta_\Sigma\zeta_{\Sigma^c}.$$

But since $\Sigma_1^{\mathrm{c}}, \Sigma_2^{\mathrm{c}}$ are disjoint we have $\zeta_{\Sigma^{\mathrm{c}}} = \zeta_{\Sigma_1^{\mathrm{c}}} + \zeta_{\Sigma_2^{\mathrm{c}}}$ by the linearity of convolution, so

$$\begin{aligned}\zeta_{\Sigma}\zeta_{\Sigma^{\mathrm{c}}} &= \big(1-\zeta_{\Sigma_1^{\mathrm{c}}}-\zeta_{\Sigma_2^{\mathrm{c}}}\big)\big(\zeta_{\Sigma_1^{\mathrm{c}}}+\zeta_{\Sigma_2^{\mathrm{c}}}\big)\\ &= \big(1-\zeta_{\Sigma_1^{\mathrm{c}}}\big)\zeta_{\Sigma_1^{\mathrm{c}}} + \big(1-\zeta_{\Sigma_2^{\mathrm{c}}}\big)\zeta_{\Sigma_2^{\mathrm{c}}} - 2\zeta_{\Sigma_1^{\mathrm{c}}}\zeta_{\Sigma_2^{\mathrm{c}}}\\ &= \big(\zeta_{\Sigma_1}\zeta_{\Sigma_1^{\mathrm{c}}} + \zeta_{\Sigma_2}\zeta_{\Sigma_2^{\mathrm{c}}}\big) - 2\zeta_{\Sigma_1^{\mathrm{c}}}\zeta_{\Sigma_2^{\mathrm{c}}}.\end{aligned}$$

But $\zeta_{\Sigma_1^{\mathrm{c}}}\zeta_{\Sigma_2^{\mathrm{c}}}$ is the integrand of R, so this completes this step.

Step 3: Bound above for R. We now show that

$$R \lesssim \int_0^\infty \int_{-\infty}^\infty \chi_{[-s,\infty)}(y-\sigma(x))\,\chi_{[-s,\infty)}(-y)\,\mathrm{d}y\,\mathrm{d}x$$

for a fixed $s>0$ that is independent of r. To do this, first note that since W is supported within $B_\ell(\mathbf{0})$ we have

$$|W(x,y)| \lesssim \chi_{B_\ell(\mathbf{0})}(x,y) \leqslant \chi_{[-\ell,\ell]}(x)\,\chi_{[-\ell,\ell]}(y).$$

The first factor in the integrand of R therefore satisfies

$$\begin{aligned}|W*\chi_{\Sigma_1^{\mathrm{c}}}(x,y)| &\lesssim \chi_{[-\ell,\ell]^2}*\chi_{\Sigma_1^{\mathrm{c}}}(x,y)\\ &= \int_{-\infty}^\infty\int_{-\infty}^\infty \chi_{(-\infty,0]}(y-v)\,\chi_{[-\ell,\ell]}(u)\,\chi_{[-\ell,\ell]}(v)\,\mathrm{d}u\,\mathrm{d}v\\ &\leqslant \int_{-\infty}^\infty\int_{-\infty}^\infty \chi_{(-\infty,\ell]}(y)\,\chi_{[-\ell,\ell]}(u)\,\chi_{[-\ell,\ell]}(v)\,\mathrm{d}u\,\mathrm{d}v\\ &= 4\ell^2\chi_{[-\ell,\infty)}(-y).\end{aligned}$$

The second factor in the integrand of R satisfies

$$\begin{aligned}|W*\chi_{\Sigma_2^{\mathrm{c}}}(x,y)| &\lesssim \chi_{[-\ell,\ell]^2}*\chi_{\Sigma_2^{\mathrm{c}}}(x,y)\\ &= \int_{-\infty}^\infty\int_{-\infty}^\infty \chi_{[0,\infty)}(y-v-\sigma(x-u))\,\chi_{[-\ell,\ell]}(u)\,\chi_{[-\ell,\ell]}(v)\,\mathrm{d}u\,\mathrm{d}v.\end{aligned}$$

But

$$\begin{aligned}y \geqslant \sigma(x-u)+v \quad &\Longrightarrow \quad y \geqslant \min_{w\in[x-\ell,x+\ell]}\sigma(w)-\ell\\ &\Longrightarrow \quad y \geqslant \sigma(x) - \ell\sup_{w\in\mathbb{R}_+}|\sigma'(w)| - \ell.\end{aligned}$$

Recalling that $\sigma(x) = r\,\omega(x/r)$, so $\sigma'(x) = \omega'(x/r)$, we find that

$$s := \ell\Big(1+\sup_{w\in\mathbb{R}_+}|\sigma'(w)|\Big)$$

is independent of r, and

$$\begin{aligned}|W*\chi_{\Sigma_2^{\mathrm{c}}}(x,y)| &\lesssim \int_{-\infty}^\infty\int_{-\infty}^\infty \chi_{[-s,\infty)}(y-\sigma(x))\,\chi_{[-\ell,\ell]}(u)\,\chi_{[-\ell,\ell]}(v)\,\mathrm{d}u\,\mathrm{d}v\\ &= 4\ell^2\chi_{[-s,\infty)}(y-\sigma(x)).\end{aligned}$$

This completes the claim made at the start of this step.

Inequality for Step 4. In the next step we will need to find a lower bound for the integral

$$I(y) = \int_{-\infty}^{\infty} \chi_{(-\infty,0]}(y-v)\,\chi_{[-2m,2m]}(v)\,\mathrm{d}v.$$

For the first indicator function in the integrand, the analogous bound to the previous step would be

$$\chi_{(-\infty,0]}(y-v) \geqslant \chi_{(-\infty,-2m]}(y),$$

which gives $I(y) \geqslant 4m\chi_{[2m,\infty)}(-y)$. However, this would end up giving a lower bound of zero for R because the two factors in its integrand would not be non-zero on any shared region. To avoid this, we note that $I(y)$ is piecewise linear (with $I(y)=0$ for $y>m$ and $I(y)=2m$ for $y<-m$) and we choose a lower bound that is non-zero even for some positive values of y. Specifically,

$$y \leqslant v, -2m \leqslant v \leqslant 2m \quad \Longleftarrow \quad y \leqslant m,\, m \leqslant v \leqslant 2m,$$

so

$$I(y) \geqslant \int_{-\infty}^{\infty} \chi_{(-\infty,m]}(y)\,\chi_{[-m,2m]}(v)\,\mathrm{d}v = m\chi_{(-\infty,m]}(y).$$

Similarly, we bound

$$\int_{-\infty}^{\infty} \chi_{[0,\infty)}(y-v-k)\,\chi_{[-2m,2m]}(v)\,\mathrm{d}v \geqslant \int_{-\infty}^{\infty} \chi_{[-m,\infty)}(y-k)\,\chi_{[-2m,-m]}(v)\,\mathrm{d}v = m\chi_{[-m,\infty)}(y-k).$$

Step 4: Bound below for R. We now show that

$$R \gtrsim \int_0^{\infty} \int_{-\infty}^{\infty} \chi_{[-t,\infty)}(y-\sigma(x))\,\chi_{[-t,\infty)}(-y)\,\mathrm{d}y\,\mathrm{d}x$$

for a fixed $t>0$ that is independent of r. We proceed in a similar way to the previous step, but some of the details are different. First note that, since W is continuous and strictly positive at $\mathbf{0}$, there exists $m>0$ such that

$$|W(x,y)| \gtrsim \chi_{[-2m,2m]}(x)\,\chi_{[-2m,2m]}(y).$$

Therefore, using the inequality proved just before this step, the first factor in the integrand of R satisfies

$$\begin{aligned}|W * \chi_{\Sigma_1^c}(x,y)| &\gtrsim \chi_{[-2m,2m]^2} * \chi_{\Sigma_1^c}(x,y)\\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \chi_{(-\infty,0]}(y-v)\,\chi_{[-2m,2m]}(u)\,\chi_{[-2m,2m]}(v)\,\mathrm{d}u\,\mathrm{d}v\\ &\geqslant 4m^2\chi_{(-\infty,m]}(y).\end{aligned}$$

For any $h \leqslant 2m$, the second factor in the integrand of R satisfies

$$\begin{aligned}|W * \chi_{\Sigma_2^c}(x,y)| &\gtrsim \chi_{[-2m,2m]^2} * \chi_{\Sigma_2^c}(x,y)\\ &\geqslant \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \chi_{[0,\infty)}(y-v-\sigma(x-u))\,\chi_{[-h,h]}(x)\,\chi_{[-2m,2m]}(y)\,\mathrm{d}u\,\mathrm{d}v.\end{aligned}$$

But

$$
\begin{aligned}
y \geqslant \sigma(x-u)+v \quad &\Longleftarrow \quad y \geqslant \max_{w\in[x-h,x+h]} \sigma(w)+v \\
&\Longleftarrow \quad y \geqslant \sigma(x)+h \sup_{w\in\mathbb{R}_+} |\sigma'(w)|+v.
\end{aligned}
$$

Using the inequality proved before this step, we find that

$$
|W * \chi_{\Sigma_2^c}(x,y)| \gtrsim 2hm\chi_{[-m,\infty)}\Big(y-\sigma(x)-h\sup_{w\in\mathbb{R}_+}|\sigma'(w)|\Big).
$$

Choosing $h \leqslant m/\big(2\sup_{w\in\mathbb{R}_+}|\sigma'(w)|\big)$, and setting $t \leqslant m/2$, proves the claim made at the start of this step.

Step 5: Bound in terms of σ^{-1}. We now show that

$$
\sigma^{-1}(t) \lesssim R \lesssim \sigma^{-1}(2s).
$$

For both bounds we must investigate the integral

$$
I := \int_0^\infty \int_{-\infty}^\infty \chi_{[-s,\infty)}(y-\sigma(x))\,\chi_{[-s,\infty)}(-y)\,\mathrm{d}y\,\mathrm{d}x
$$

(with t in place of s for the lower bound). This integrand is 1 if and only if $\sigma(x)-s \leqslant y$ and $y \leqslant s$ both hold (in particular, $\sigma(x) \leqslant 2s$), so evaluating the $\mathrm{d}y$ integral we find

$$
I = \int_0^\infty (2s-\sigma(x))\,\chi_{(-\infty,2s]}(\sigma(x))\,\mathrm{d}x.
$$

We have $2s-\sigma(x) \leqslant 2s$, and the integrand is non-zero if and only if $\sigma(x) \leqslant 2s$ i.e. $x \leqslant \sigma^{-1}(2s)$, so

$$
I \leqslant 2s \int_0^{\sigma^{-1}(2s)} \mathrm{d}x = 2s\sigma^{-1}(2s).
$$

For the lower bound we note that $1 \geqslant \chi_{(-\infty,t]}(\sigma(x))$, which is non-zero when $\sigma(x) \leqslant t$ i.e. $x \leqslant \sigma^{-1}(t)$ and $2t-\sigma(x) \geqslant t$, so

$$
\begin{aligned}
I &\geqslant \int_0^\infty (2t-\sigma(x))\,\chi_{(-\infty,t]}(\sigma(x))\,\chi_{(-\infty,2t]}(\sigma(x))\,\mathrm{d}x \\
&= \int_0^\infty (2t-\sigma(x))\,\chi_{(-\infty,t]}(\sigma(x))\,\mathrm{d}x \\
&\geqslant t \int_0^{\sigma^{-1}(t)} \mathrm{d}x = t\sigma^{-1}(t).
\end{aligned}
$$

Step 6: Asymptotic expression for R. Recall that $\sigma(x) = r\omega(x/r)$, so $\sigma^{-1}(s) = \omega^{-1}(rs)/r$; to see this, note that if $s = \sigma(x)$ then

$$
r\omega^{-1}(s/r) = r\omega^{-1}(r\omega(x/r)/r) = x = \sigma^{-1}(s).
$$

We have therefore shown that

$$
r\omega^{-1}(s/r) \lesssim R \lesssim r\omega^{-1}(t/r).
$$

We will use this to show that $R = \Theta(r\omega^{-1}(1/r))$, which completes the proof.

We first prove an inequality for ω^{-1}. By assumption, ω is convex close to 0, which implies that $\omega(\alpha y) \leqslant \alpha\omega(y)$ for all sufficiently small y and every $0 \leqslant \alpha \leqslant 1$. For all sufficiently small v, putting $y := \omega^{-1}(v)$, we find that

$$\alpha\omega^{-1}(v) = \alpha y \leqslant \omega^{-1}(\alpha\omega(y)) = \omega^{-1}(\alpha v).$$

For $t \geqslant 1$ we may apply this with $\alpha = 1/t$ giving

$$r\omega^{-1}\left(\frac{t}{r}\right) \leqslant r\,t\,\omega^{-1}\left(\frac{1}{t}\frac{t}{r}\right) = r\,t\,\omega^{-1}\left(\frac{1}{r}\right),$$

while for $t \leqslant 1$ we may use the fact that ω^{-1} is increasing close to 0 to give

$$r\omega^{-1}\left(\frac{t}{r}\right) \leqslant \omega^{-1}\left(\frac{1}{r}\right).$$

For the lower bound, we apply the inequalities the opposite way round: for $s \geqslant 1$ we note that

$$r\omega^{-1}\left(\frac{s}{r}\right) \geqslant r\omega^{-1}\left(\frac{1}{r}\right),$$

while for $s \leqslant 1$ we have

$$r\omega^{-1}\left(\frac{s}{r}\right) \geqslant r\,s\,\omega^{-1}\left(\frac{1}{r}\right).$$

This proves that $R = \Theta(r\omega^{-1}(1/r))$. $\square$

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