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Semi-classical analysis and pseudo-spectra

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Abstract

We prove an approximate spectral theorem for non-self-adjoint operators and investigate its applications to second-order differential operators in the semi-classical limit. This leads to the construction of a twisted FBI transform. We also investigate the connections between pseudo-spectra and boundary conditions in the semi-classical limit.

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1. Introduction

In the last ten years the theory of pseudo-spectra has developed rapidly, and has been shown to give substantial insights into the properties of non-self-adjoint (NSA) matrices and operators [1,5,7,11,22,23]. In this paper we focus on its applications to second-order differential operators. This involves giving a new and more general definition of pseudo-spectra. Our first reason for extending the concept is that the standard definition does not provide any link with the geometry of phase space, which is of great importance in the theory of differential and pseudo-differential operators. By incorporating the connection into the definitions, we increase the conceptual clarity and

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facilitate the analysis of pseudo-spectra in those situations in which the semi-classical approximation is relevant.

The second reason for concentrating on pseudo-eigenfunctions rather than pseudo-spectra is that the former are used in [6] to provide a new method of solving evolution equations approximately. In several dimensions one could not hope to obtain sufficient pseudo-eigenfunctions by choosing just one for each point of the complex plane. Questions of spectral multiplicity arise just as they do for ordinary spectral theory, and indicate that a better parameterization is by points in the classical phase space, not by complex numbers. We plan to use the results of this paper to extend those of [6] to more general operators.

The paper has three parts. In the first we prove an abstract approximate spectral theorem for NSA operators. We find a connection between this and quantization. The second part relates these ideas to the semi-classical analysis of differential operators via the semi-classical principal symbol of the operator and what we call interior pseudo-eigenvectors. Finally, we introduce the concept of boundary pseudo-eigenvectors and describe how to construct them. We mention that [24] contains results relating the boundary and interior pseudo-spectra of twisted Toeplitz operators which are parallel to the ones which we obtain for differential operators. See [9] for related work on the wave equation.

2. An approximate spectral theorem

In [6] we have shown how to 'diagonalize' highly non-normal operators by using pseudo-spectra. The diagonalization is only approximate, but, in spite of this, it may be used to solve evolution equations efficiently for some quite singular infinitesimal generators.

In this paper, we formulate the underlying theorem at a general level, in order to make it accessible to a wider audience. All the assumptions here are satisfied in the numerical examples discussed in [6], as we indicate in the next section. The ingredients are simple. We suppose that A is a bounded or closed, unbounded linear operator acting in a separable Hilbert space $\mathscr{H}$. We also suppose that Λ is a multiplication operator acting in the space $L^p(\Omega, \mathrm{d}\omega)$ where $1 \leqslant p < \infty$; for numerical calculations the simplest choice is $p = 2$, but $p = 1$ is more natural for some other purposes. We assume explicitly that

$$(\Lambda\psi)(\omega) = \sigma(\omega)\psi(\omega)$$

for all ψ in the maximal subdomain of $L^p(\Omega)$, where the 'symbol' $\sigma : \Omega \to \mathbf{C}$ of the operator A is a measurable function and $\mathrm{d}\omega$ is a σ-finite measure on Ω. It is known that the spectrum of the operator Λ equals the essential range of σ. We also assume that $E : L^p(\Omega) \to \mathscr{H}$ is a bounded linear operator such that $E(\mathrm{Dom}(\Lambda)) \subseteq \mathrm{Dom}(A)$ and that

$$\|AE - E\Lambda\| < \varepsilon \tag{1}$$

for a (preassigned, small) $\varepsilon > 0$, in the sense that

$$\|AE\phi - E\Lambda\phi\| < \varepsilon\|\phi\| \tag{2}$$

for all $\phi \in \mathrm{Dom}(\Lambda)$.

Theorem 1. *Let A be the generator of a one-parameter semi-group T_t acting on $\mathscr{H}$ and satisfying*

$$\|T_t\| \leqslant M e^{\gamma t} \tag{3}$$

for all $t \geqslant 0$. Suppose also that

$$\mathrm{Re}(\sigma(\omega)) \leqslant \gamma$$

for all $\omega \in \Omega$. Then (1) *implies*

$$\|T_t E - E e^{\Lambda t}\| \leqslant \varepsilon t M e^{\gamma t} \tag{4}$$

for all $t \geqslant 0$.

Proof. Since the operators in (4) are all bounded it is sufficient to prove the estimate for all $\phi \in \mathrm{Dom}(\Lambda)$. We then have

$$\begin{aligned}
\|T_t E\phi - E e^{\Lambda t}\phi\| &= \left\| \int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\left(T_{t-s} E e^{\Lambda s}\phi\right) \mathrm{d}s \right\| \\
&\leqslant \int_0^t \|T_{t-s}(AE - E\Lambda) e^{\Lambda s}\phi\| \,\mathrm{d}s \\
&\leqslant \int_0^t \|T_{t-s}\|\varepsilon\|e^{\Lambda s}\phi\| \,\mathrm{d}s \\
&\leqslant \int_0^t M e^{\gamma(t-s)}\varepsilon e^{\gamma s}\|\phi\| \,\mathrm{d}s \\
&= \varepsilon\|\phi\| t M e^{\gamma t}. \quad \square
\end{aligned}$$

If A is a bounded normal operator then the spectral theorem states that one can find such a representation in which E is unitary, $\varepsilon = 0$ and the essential range of Λ equals the spectrum of A. The point of Theorem 1 is that it may be applied to operators which are far from unitary and in situations in which the essential range of Λ is very different from the spectrum of A. The explanation of this relates to pseudo-spectral theory.

One might try to develop an ‘approximate functional calculus’ based upon the above theorem. For example, if $T_t = \mathrm{e}^{At}$ is a contraction semi-group then under suitable conditions one can prove an analogue of Theorem 1 for $T_{\alpha,t} = \mathrm{e}^{-(-A)^{\alpha}t}$ when $0 < \alpha < 1$; see [6].

In order to compare Theorem 1 with the results in [6] one needs to approximate E by an operator E' whose range is not contained in $\mathrm{Dom}(A)$.

Corollary 2. *If in addition to the previous assumptions one has* $\|E - E'\| < \varepsilon$ *then*

$$\|T_t E'\phi - E'\mathrm{e}^{\Lambda t}\phi\| \leqslant \varepsilon\|\phi\|(1 + M + tM)\mathrm{e}^{\gamma t} \tag{5}$$

for all $\phi \in L^p(\Omega)$ *and all* $t \geqslant 0$.

Proof. This follows directly from

$$\begin{aligned}\|T_t E'\phi - E'\mathrm{e}^{\Lambda t}\phi\| \;\leqslant\; & \|T_t E\phi - E\mathrm{e}^{\Lambda t}\phi\| \\ & + \|T_t(E - E')\phi\| + \|(E - E')\mathrm{e}^{\Lambda t}\phi\|. \qquad \square\end{aligned}$$

The following modification of Theorem 1 assumes that one is given $f \in \mathscr{H}$ and wishes to approximate $T_t f$.

Corollary 3. *If* $f \in \mathscr{H}$ *then under the conditions of Theorem* 1

$$\|T_t f - E\mathrm{e}^{\Lambda t}\phi\| \leqslant \|f - E\phi\| M\mathrm{e}^{\gamma t} + \varepsilon\|\phi\| tM\mathrm{e}^{\gamma t}$$

for all $\phi \in L^p(\Omega)$ *and* $t \geqslant 0$.

Proof. We have

$$\|T_t f - E\mathrm{e}^{\Lambda t}\phi\| \leqslant \|T_t(f - E\phi)\| + \|T_t E\phi - E\mathrm{e}^{\Lambda t}\phi\|$$

each of which is straightforward to estimate. $\square$

The above results can only be useful if M, t and γ are of order 1. There also has to exist ϕ such that $\|f - E\phi\|$ and $\varepsilon\|\phi\|$ are small. One cannot simply put $\phi = E^{-1}f$, since E need not be surjective or invertible.

If $p = 2$, the standard way of solving this problem is to minimize the functional

$$\mathscr{E}(\phi) = \|f - E\phi\|^2 + \delta\|\phi\|^2 \tag{6}$$

for a suitable value of the regularization parameter $\delta > 0$; see [12]. This is achieved in the numerical context by putting

$$\phi = \tilde{E}\backslash(f \oplus 0),$$

where $\tilde{E} : L^2(\Omega) \to \mathscr{H} \oplus L^2(\Omega)$ is defined by

$$\tilde{E}\phi = E\phi \oplus \delta^{1/2}\phi. \tag{7}$$

Also $x = G\backslash g$ is the Matlab notation for the best approximate solution x of a possibly singular linear equation $Gx = g$.

We include the proof of the following well-known proposition for completeness.

Proposition 4. *If $p = 2$, the minimum of* (6) *is achieved for $\phi = F_\delta f$, where*

$$F_\delta = (E^*E + \delta I)^{-1}E^* \tag{8}$$

satisfies $\|F_\delta\| \leqslant \delta^{-1/2}$. Moreover $\|EF_\delta\| \leqslant 1$ for all $\delta > 0$. One has

$$\lim_{\delta \to 0} EF_\delta f = f \tag{9}$$

for all $f \in \mathscr{H}$ if and only if $\mathrm{Ran}(E)$ *is dense in $\mathscr{H}$.*

Proof. The first statement depends upon a routine variational calculation. For the second we observe that

$$\|(E^*E + \delta I)^{-1}E^*\| \leqslant ab,$$

where

$$a = \|(E^*E + \delta I)^{-1/2}\| \leqslant \delta^{-1/2}$$

and

$$\begin{aligned} b^2 &= \|(E^*E + \delta I)^{-1/2}E^*\|^2 \\ &= \|(E^*E + \delta I)^{-1/2}E^*. E(E^*E + \delta I)^{-1/2}\| \\ &\leqslant \|(E^*E + \delta I)^{-1/2}(E^*E + \delta I)(E^*E + \delta I)^{-1/2}\| \\ &= 1. \end{aligned}$$

This calculation also implies that

$$\begin{aligned} \|EF_\delta\| &= \|E(E^*E + \delta I)^{-1/2}. (E^*E + \delta I)^{-1/2}E^*\| \\ &= \|(E^*E + \delta I)^{-1/2}E^*\|^2 \\ &\leqslant 1. \end{aligned}$$

Since $\mathrm{Ran}(EF_\delta) \subseteq \mathrm{Ran}(E)$, (9) implies that $\mathrm{Ran}(E)$ is dense. If $\mathrm{Ran}(E)$ is dense then the uniform boundedness just proved implies that (9) holds for all $f \in \mathscr{H}$ if it holds whenever $f = E\phi$ for some $\phi \in L^2(\Omega)$. In this case let P denote the orthogonal projection onto the closure of the range of E^*E. Since $\mathrm{Ker}(E) = \mathrm{Ker}(E^*E)$, we may assume without loss of generality that $P\phi = \phi$. We have

$$\lim_{\delta\to 0} EF_\delta f = \lim_{\delta\to 0} E(E^*E + \delta I)^{-1}E^*E\phi$$
$$= EP\phi = E\phi = f$$

by applying the spectral theorem to the non-negative self-adjoint operator E^*E. $\square$

Using Proposition 4 one may ensure that $\varepsilon\|\phi\|$ is small by choosing δ appropriately. Even if E has dense range, one cannot ensure that $\|f - E\phi\|$ is small for some particular $\delta > 0$ without further conditions. One has either to make the a priori assumption that f lies in some subspace of well-approximable vectors, or observe a posteriori for particular choices of f and δ that the minimizing ϕ does indeed make this quantity small enough for the application intended.

3. The connection with pseudo-spectra

Given $\varepsilon > 0$, the ε-pseudo-spectrum of the closed operator A is defined by

$$\mathrm{Spec}_\varepsilon(A) = \mathrm{Spec}(A) \cup \{z : \|Af - zf\| < \varepsilon\|f\| \text{ for some } f \in \mathrm{Dom}(A)\}.$$

Pseudo-spectral ideas lie at the core of this paper, and we refer to [1,5,7,11,22,23] for background material on this subject. The following theorem is valid for all $p \in [1, \infty)$, but its main application is for $p = 1$. Indeed we conjecture that if $p = 2$ the first condition on E can only hold if E is isometric. In the following theorem P_U denotes the operator of multiplication by the characteristic function of the set U, always assumed to be measurable.

Theorem 5. *Suppose that $1 \leqslant p < \infty$, $\|EP_U\| = 1$ for all subsets U of Ω with positive measure, and $\|AE - E\Lambda\| < \varepsilon$. Then*

$$\mathrm{Spec}(\Lambda) \subseteq \mathrm{Spec}_\varepsilon(A).$$

Proof. Let $\beta \in \mathrm{Spec}(\Lambda)$. We choose $\delta > 0$ such that

$$\varepsilon' := \|AE - E\Lambda\| + \delta < \varepsilon$$

and put

$$U = \{\omega \in \Omega : |\sigma(\omega) - \beta| < \delta\}.$$

If ϕ has support in U then

$$\begin{aligned} \|AE\phi - \beta E\phi\| &\leqslant \|(AE - E\Lambda)\phi\| + \|E(\Lambda\phi - \beta\phi)\| \\ &\leqslant \varepsilon'\|\phi\|. \end{aligned}$$

Therefore,

$$\begin{aligned} \inf\{\|Af - \beta f\|/\|f\| : 0 \neq f \in \mathscr{H}\} &\leqslant \inf\{\|AE\phi - \beta E\phi\|/\|E\phi\| : 0 \neq \phi \in L^p(U)\} \\ &\leqslant \varepsilon' \inf\{\|\phi\|/\|E\phi\| : 0 \neq \phi \in L^p(U)\} \\ &= \varepsilon' < \varepsilon. \end{aligned}$$

This implies that $\beta \in \mathrm{Spec}_\varepsilon(A)$. □

Theorem 6. *Suppose that for each $\omega \in \Omega$ there is a unit vector $e_\omega \in \mathrm{Dom}(A)$ which depends measurably on ω, and define $E : L^1(\Omega) \to \mathscr{H}$ by*

$$Ef = \int_\Omega f(\omega)e_\omega \,\mathrm{d}\omega.$$

Then the conditions of Theorem 5 *hold if and only if there exists $\varepsilon' > 0$ and a set N of zero measure such that*

$$\|Ae_\omega - \sigma_\omega e_\omega\| \leqslant \varepsilon' < \varepsilon$$

for all $\omega \in \Omega \backslash N$, where $\sigma(\omega) \in \mathbf{C}$.

Proof. The passage from the assumptions of Theorem 5 to the statements of this theorem is justified by using [10, Theorem VI.8.6]. □

If ϕ lies in the maximal domain of Λ then under the assumptions of Theorem 6

$$\|AE\phi - E\Lambda\phi\| \leqslant \int_\Omega |\phi(\omega)|\, \|Ae_\omega - \sigma_\omega e_\omega\| \,\mathrm{d}\omega \leqslant \varepsilon'\|\phi\|. \tag{10}$$

Hence $\|AE - E\Lambda\| \leqslant \varepsilon' < \varepsilon$. The calculations involved would be easy to justify if one only had to deal with finite sums, or if A and Λ were bounded, but in general they use limiting processes to define the integrals. Commuting A and Λ with these limiting processes is justified by the following lemma.

Lemma 7. *Let A be a closed linear operator with domain in a Banach space $\mathscr{B}$ and range in a Hilbert space $\mathscr{H}$. Let $c > 0$, $f_n \in \mathrm{Dom}(A)$, $\|f_n - f\| \to 0$, $\|g_n - g\| \to 0$ and $\|Af_n - g_n\| \leqslant c$ for all n, then $f \in \mathrm{Dom}(A)$ and $\|Af - g\| \leqslant c$.*

Proof. By applying the Hahn–Banach theorem to the graph of A we see that it is also weakly closed. Under the stated assumptions we have $\|Af_n - g\| \leqslant c + 1$ for all large enough n. By the weak compactness of all closed balls in $\mathscr{H}$, there is a subsequence $f_{n(r)}$ such that $Af_{n(r)}$ converges weakly as $r \to \infty$. Denoting the limit by h, the equations $\|f_{n(r)} - f\| \to 0$ and $Af_{n(r)} \to h$ weakly as $r \to \infty$ imply that $f \in \mathrm{Dom}(A)$ and $Af = h$. Since

$$Af_{n(r)} - g_{n(r)} \to Af - g$$

weakly as $r \to \infty$ and $\|Af_{n(r)} - g_{n(r)}\| \leqslant c$ for all r, we conclude that $\|Af - g\| \leqslant c$.

If Ω has finite measure $|\Omega|$, then $L^2(\Omega)$ is continuously embedded in $L^1(\Omega)$, and all of the theorems of Section 1 hold under the present hypotheses. In the numerical applications of [6] the space Ω is taken to be the finite set $\{1, \ldots, N\}$ and $\mathrm{d}\omega$ is the counting measure. Given unit pseudo-eigenvectors $e_n \in \mathscr{H}$ of A for $1 \leqslant n \leqslant N$, we have

$$E\phi = \sum_{n=1}^{N} \phi_n e_n. \tag{11}$$

There is no requirement that the vectors should be linearly independent, and indeed in some of the examples studied in [6] they are taken from an overcomplete infinite sequence $\{e_n\}_{n=1}^{\infty}$. Equivalently the operator E need not be invertible, or may have a large condition number.

4. Quantization

In this section, we make some general comments about the relationship between our previous results and the notion of quantization.

Let Ω be a second countable locally compact Hausdorff space, and let $\mathrm{d}\omega$ be a regular Borel measure on Ω with support equal to Ω. Let $\mathscr{H}$ be a separable Hilbert space and let $e : \Omega \to \mathscr{H}$ be a continuous function. We define $E : C_c(\Omega) \to \mathscr{H}$ by

$$E\phi = \int_\Omega \phi(\omega) e_\omega \, \mathrm{d}\omega.$$

The following are well-known and elementary.

Lemma 8. *The operator E extends to a bounded linear operator $E_1 : L^1(\Omega, \mathrm{d}\omega) \to \mathscr{H}$ if and only if $\omega \to \|e_\omega\|$ is a bounded function, in which case*

$$\|E_1\| = \sup\{\|e_\omega\| : \omega \in \Omega\}.$$

The operator E extends to a bounded linear operator $E_2 : L^2(\Omega, \mathrm{d}\omega) \to \mathscr{H}$ if and only if

$$\int_\Omega |\langle f, e_\omega\rangle|^2 \,\mathrm{d}\omega \leqslant c^2 \|f\|^2 \tag{12}$$

for some $c \geqslant 0$ and all $f \in \mathscr{H}$, in which case $\|E_2\|$ is the smallest such constant c. The operator $E^* : \mathscr{H} \to C(\Omega)$ is an isometry from $\mathscr{H}$ into $L^2(\Omega, \mathrm{d}\omega)$ if and only if

$$\int_\Omega |\langle f, e_\omega\rangle|^2 \,\mathrm{d}\omega = \|f\|^2 \tag{13}$$

for all $f \in \mathscr{H}$.

Families of vectors $\{e_\omega\}_{\omega\in\Omega}$ satisfying (13) are also called continuous resolutions of the identity and have played an important part in group representation theory and quantum mechanics for many decades. For their connection with coherent state theory and the Bargman transform see [2, Chapter 8] and [17, Chapter 3]. If (13) holds then $E\backslash f = E^* f$ for all $f \in \mathscr{H}$, but this is not the case under assumption (12), which is more relevant to this paper.

Given a function $f \in C_c(\Omega)$ we define the multiplication operator M_f by $M_f\phi = f\phi$ where $\phi \in L^p(\Omega)$ for some p. We define the quantization of the function f to be the operator $Q(f) = EM_fE^*$ on $\mathscr{H}$. We may also write

$$Q(f) = \int_\Omega f(\omega) P_{e_\omega} \,\mathrm{d}\omega,$$

where $P_a\psi = \langle\psi, a\rangle a$; see, for example, [2, Section 8.5]. The following lemma is also standard.

Lemma 9. *If $f \geqslant 0$ then $Q(f) \geqslant 0$. If E is bounded from $L^1(\Omega)$ to $\mathscr{H}$ then Q extends to a bounded linear operator from $L^1(\Omega)$ to the space $\mathscr{T}(\mathscr{H})$ of trace class operators on $\mathscr{H}$. If E is bounded from $L^2(\Omega)$ to $\mathscr{H}$ then Q extends to a bounded linear operator from $L^\infty(\Omega)$ to the space $\mathscr{L}(\mathscr{H})$ of bounded operators on $\mathscr{H}$. Given* (13), *or equivalently $EE^* = 1$, we have $Q(1) = 1$.*

In quantum theory it is commonplace to refer not to the operator Q but to the positive-operator-valued measure $A(U) := EM_{\chi_U}E^*$ where χ_U is the characteristic function of the measurable set U of Ω. The formula

$$Q(f) = \int_\Omega f(\omega) A(\mathrm{d}\omega)$$

implements a one–one correspondence between the two definitions; see [2, Lemma 3.1.2]. If $EE^* = 1$ then $A(\Omega) = 1$ and $A(\cdot)$ is called a generalized observable; for a systematic study of POV measures and their relation to coherent states see [2, Chapter 3] or [15]. See [13] for more recent references and a connection with subnormal operators.

The difference between this method of quantization and the approach of this paper is now clear. Instead of studying $Q(f) = EM_f E^*$, we would like to study $S(f) = EM_f E^{-1}$. If this were possible $f \to S(f)$ would be an algebra homomorphism from $L^\infty(\Omega)$ to $\mathscr{L}(\mathscr{H})$. Since E is not invertible in general we compromise by studying $EM_f F_\delta$, where the regularized inverse F_δ is given by (8) and $\delta > 0$ is chosen small enough to yield numerically valuable results but not so small that the computational algorithms become unreliable.

The operator E which we have considered above has much in common with the Fourier–Bros–Iagolnitzer (FBI) transform as defined in [17, Chapter 3]. See also [2, Chapter 3], where the connection with the Wigner distribution and applications to quantum theory are explained. In Section 8, we define a distorted FBI transform; the distortions are introduced to adapt the transform to a given differential operator, and involve replacing the Gaussian states used in the definition of the FBI transform by pseudo-eigenfunctions of the operator.

5. The connection with semi-classical analysis

Before describing the connection of the above ideas with semi-classical analysis, we generalize the notion of pseudo-spectra. Following [7,14,16,21], we define the (generalized) pseudo-spectra of a family of closed operators $\{A_\omega\}_{\omega\in\Omega}$ acting from dense domains $\mathrm{Dom}(A_\omega)$ in a Banach space $\mathscr{B}$ to another Banach space $\mathscr{C}$ to be the sets

$$\mathrm{Spec}_\varepsilon(A) = \{\omega : \|A_\omega f\| < \varepsilon\|f\| \text{ for some } f \in \mathrm{Dom}(A_\omega)\},$$

where $\varepsilon > 0$. Note our unorthodox omission of $\mathrm{Spec}(A)$ in this definition, explained below. We have

$$\mathrm{Spec}_\varepsilon(A) \cup \mathrm{Spec}_\varepsilon(A^*) = \mathrm{Spec}(A) \cup \left\{\omega : \|A_\omega^{-1}\| > \varepsilon^{-1}\right\},$$

where $\mathrm{Spec}(A)$ is defined to be the set of ω for which A_ω is not invertible. If $\dim(\mathscr{B}) = \dim(\mathscr{C}) < \infty$ then

$$\mathrm{Spec}(A) \subseteq \mathrm{Spec}_\varepsilon(A) = \mathrm{Spec}_\varepsilon(A^*)$$

for all $\varepsilon > 0$. If $\dim(\mathscr{B}) < \dim(\mathscr{C}) < \infty$ then

$$\mathrm{Spec}_\varepsilon(A^*) = \mathrm{Spec}(A) = \Omega$$

for all $\varepsilon > 0$, but $\mathrm{Spec}_\varepsilon(A)$ may nevertheless be an interesting set. The proof of the following lemma may be found in [14].

Lemma 10. *One has* $\omega \in \mathrm{Spec}_\varepsilon(A)$ *if and only if there exists a bounded operator* $D : \mathscr{B} \to \mathscr{C}$ *such that* $\|D\| < \varepsilon$ *and*

$$\mathrm{Ker}(A(\omega) + D) \neq \{0\}.$$

Given a differential or pseudo-differential operator L_h with domain $C_c^\infty(X)$, where X is a region in $\mathbf{R}^N$ and $h > 0$, we define the operator family

$$A_{h,u,\xi} : C_c^\infty(X) \subseteq L^2(X) \to L^2\left(X, \mathbf{C}^{2N+1}\right)$$

by

$$A_{h,u,\xi} f = (Q^j f - u^j f, P_j f - \xi_j f, L_h f - \sigma(u, \xi) f), \tag{14}$$

where $(Q^j f)(x) = x^j f(x)$ and $(P_j f)(x) = -ih\partial_j f(x)$. In these equations we assume that $u \in X$, $\xi \in \mathbf{R}^N$, $1 \leqslant j \leqslant N$ and $\sigma(u, \xi)$ is the semi-classical principal symbol of the operator L_h, as defined below. It follows directly from the definitions that $\|A_{h,u,\xi} f\| < \varepsilon \|f\|$ implies

$$\begin{aligned} \|Q^j f - u^j f\| &< \varepsilon \|f\|, \\ \|P_j f - \xi_j f\| &< \varepsilon \|f\|, \\ \|L_h f - \sigma(x, \xi) f\| &< \varepsilon \|f\|, \end{aligned}$$

where $1 \leqslant j \leqslant N$. It is known that the pseudo-spectra converge to fill a certain set $\sigma(\Lambda)$ if $h \to 0$ and $\varepsilon \to 0$ simultaneously at suitable rates; see Section 7 for details. Even in one space dimension a point in $\sigma(\Lambda)$ may be the image of more than one point in Λ, so $\sigma(\Lambda)$ may have hidden structure as a subset of $\mathbf{C}$. This observation applies with less precision to the numerically determined pseudo-spectra for fixed $h > 0$ and $\varepsilon > 0$.

The extension of the above ideas to a manifold X needs some care, since the full symbol $\sigma_h(u, \xi)$ is not an invariant object in general. It is shown in [20] that one can resolve these problems if the manifold is provided with a linear connection, as happens if it is Riemannian. The symbol $\sigma_h(u, \xi)$ is then definable as a function on the cotangent bundle T^*X and Λ is a certain subset of T^*X. We do not actually need the full symbol for our problem: its semi-classical limit is sufficient. The semi-classical principal symbol is given by

$$\sigma(u, \xi) = \lim_{h \to 0} \sigma_h(u, h^{-1}\xi)$$

and is an invariant quantity, i.e. as a function on the cotangent bundle T^*X it does not depend on the choice of local coordinates.

The following alternative definition of the semi-classical principal symbol of L_h makes its invariant character clear. Suppose that $u \in X$ and ξ is a cotangent vector at u. Let f be any smooth function on X such that $\mathrm{d}f(u) = \xi$. Then

$$\sigma(u, \xi) = \left\{ \lim_{h\to 0} \mathrm{e}^{-ih^{-1}f} L_h \left(\mathrm{e}^{ih^{-1}f} \right) \right\} (u).$$

6. The semi-classical spectrum

The theory which we shall describe can be developed at several levels of generality, and in this section we consider only second-order differential operators acting on $\mathbf{R}^N$.

Given $h > 0$, let L_h denote the operator

$$(L_h f)(x) = -h^2 a_h^{j,k}(x)\partial_{j,k} f(x) - ihb_h^j(x)\partial_j f(x) + c_h(x) f(x)$$

acting on functions $f : \mathbf{R}^N \to \mathbf{C}$, where a, b, c are sufficiently regular functions whose values are, respectively, matrices, vectors and scalars with complex-valued entries, and we use the standard summation convention. Under conditions which we shall impose the domain of L_h will contain $C_c^\infty(\mathbf{R}^N)$. All considerations in this paper are local, so no growth bounds at infinity on the coefficients are needed. We allow the coefficients to be h-dependent so that the class of differential operators is invariant under local changes of coordinates. The semi-classical principal symbol of this operator is the complex-valued function

$$\sigma(u, \xi) = a_0^{j,k}(u)\xi_j\xi_k + b_0^j(u)\xi_j + c_0(u) \tag{15}$$

in which we take u, ξ to be *real* vectors in $\mathbf{R}^N$.

Given $(u, \xi) \in \mathbf{R}^N \times \mathbf{R}^N$ we are interested in finding localized approximate eigenfunctions for the operator L_h. We require that they become asymptotically exact as $h \to 0$.

Our first theorem provides the motivation for defining the semi-classical spectrum of L_h to be the set $\sigma\left(\mathbf{R}^N \times \mathbf{R}^N\right)$.

Theorem 11. *Suppose that $a_h^{j,k}(x)$, $b_h^j(x)$ and $c_h(x)$ are all locally Lipschitz continuous in $x \in \mathbf{R}^N$ and $h \in [0, 1]$, then for every $u \in \mathbf{R}^N$, $\xi \in \mathbf{R}^N$ and $h \in (0, 1]$ there exists $f_h \in C_c^\infty(\mathbf{R}^N)$ such that*

$$\|f_h\|_2 = c > 0, \tag{16}$$

$$\|Q^j f_h - u^j f_h\|_2 = O\left(h^{1/2}\right), \tag{17}$$

$$\|P_j f_h - \xi_j f_h\|_2 = O\left(h^{1/2}\right), \tag{18}$$

$$\|L_h f_h - \sigma(x,\xi) f_h\|_2 = O\left(h^{1/2}\right) \tag{19}$$

as $h \to 0$, *for all* $1 \leqslant j \leqslant N$.

Proof. Let ϕ be a non-negative C^∞ function on $\mathbf{R}^N$ which equals 1 if $|x| \leqslant 1$ and 0 if $|x| \geqslant 2$. Given $(u,\xi) \in \mathbf{R}^N \times \mathbf{R}^N$, $h > 0$ and $\alpha = 1/2$ define

$$f_h(x) = h^{-N\alpha/2} \mathrm{e}^{ih^{-1}\xi\cdot x} \phi(h^{-\alpha}(x-u)).$$

The first three statements of the theorem are routine verifications performed by the same method as follows:

We verify (19) by using the expansion

$$L_h f_h - \sigma(u,\xi) f_h = g + r_1 + r_2 + r_3 + r_4,$$

where

$$\begin{aligned} g(x) = &\left\{a_h^{j,k}(x) - a_0^{j,k}(u)\right\} \xi_j \xi_k f_h(x) \\ &+ \left\{b_h^j(x) - b_0^j(u)\right\} \xi_j f_h(x) + \{c_h(x) - c_0(u)\} f_h(x) \end{aligned}$$

and

$$\begin{aligned} r_1 &= -ih^{1-\alpha-N\alpha/2} a^{j,k}(x) \xi_j \mathrm{e}^{ih^{-1}\xi\cdot x} \phi_k(h^{-\alpha}(x-u)), \\ r_2 &= -ih^{1-\alpha-N\alpha/2} a^{j,k}(x) \xi_k \mathrm{e}^{ih^{-1}\xi\cdot x} \phi_j(h^{-\alpha}(x-u)), \\ r_3 &= h^{2-2\alpha-N\alpha/2} a^{j,k}(x) \mathrm{e}^{ih^{-1}\xi\cdot x} \phi_{j,k}(h^{-\alpha}(x-u)), \\ r_4 &= -ih^{1-\alpha-N\alpha/2} b^j(x) \xi_j \mathrm{e}^{ih^{-1}\xi\cdot x} \phi_j(h^{-\alpha}(x-u)). \end{aligned}$$

In these identities the subscripts on ϕ denote partial derivatives. The Lipschitz assumptions on the coefficients of L_h and the fact that the support of f_h has diameter of order h^α imply that

$$\|g\|_2 = O(h^\alpha)$$

as $h \to 0$. We also have $\|r_j\|_2 = O(h^{1-\alpha})$ for $j = 1, 2, 4$ and $\|r_3\|_2 = O(h^{2-2\alpha})$. The overall error is minimized by putting $\alpha = 1/2$. $\square$

7. Constructing the interior pseudo-spectra

The material in this section is based upon the fact that if the coefficients are sufficiently smooth then estimate (19) can be greatly improved by a suitable choice of f_h. In the language of Section 5 we replace (14) by

$$A_{h,u,\xi} f = \left(Q^j f - u^j f, P_j f - \xi_j f, h^{-n} \{ L_h f - \sigma_0(u, \xi) f \} \right), \tag{20}$$

where $n > 0$. The size of n depends upon the smoothness of the coefficients, which for simplicity we assume to be C^∞. The pseudo-spectral estimate $\|A_{h,u,\xi} f\| < \varepsilon \|f\|$ then implies

$$\begin{aligned} \|Q^j f - u^j f\| &< \varepsilon \|f\|, \\ \|P_j f - \xi_j f\| &< \varepsilon \|f\|, \\ \|L_h f - \sigma(x, \xi) f\| &< h^n \varepsilon \|f\|, \end{aligned}$$

where $1 \leqslant j \leqslant N$. We repeat the calculations of [3,4] for a more general second-order ordinary differential operator for completeness. The extension to pseudo-differential operators in higher dimensions, [8,25], cannot be formulated in exactly the same manner: there can be infinitely many different pseudo-eigenfunctions associated with a point in phase space, and the correct parameterization of these is not obvious. We assume that

$$(L_h f)(x) = -h^2 a(x) f''(x) - ihb(x) f'(x) + c(x) f(x)$$

so that the semi-classical principal symbol is

$$\sigma(u, \xi) = a(u)\xi^2 + b(u)\xi + c(u).$$

We assume ellipticity, in other words that $a(x) \neq 0$ for all $x \in \mathbf{R}$. Given $u, \xi \in \mathbf{R}$, we put

$$f(u + s) = h^{-1/4} \chi(s) \exp(\psi(s)) \tag{21}$$

for all $s \in \mathbf{R}$, where $\chi \in C_c^\infty$ satisfies $\chi(s) = 1$ if $|s| \leqslant \delta/2$ and $\chi(s) = 0$ if $|s| \geqslant \delta$, and $\delta > 0$ must be small enough; see the proof of Lemma 12. We assume that

$$\psi(s) = \sum_{m=-1}^{n} h^m \psi_m(s) \tag{22}$$

for some integer $n \geqslant -1$. This is a non-standard form of the JWKB expansion, and has the feature that the function f does not vanish within the interval of interest. A direct computation shows that

$$L_h f - \sigma(u, \xi) f = \left(\sum_{m=0}^{2n+2} h^m \phi_m \right) f + \mathrm{Rem}, \tag{23}$$

where $\mathrm{Rem} = O(h^\infty)$ as $h \to 0$ under the conditions which we impose below. Also

$$\begin{aligned} \phi_0(s) &= -a(u+s)(\psi'_{-1}(s))^2 - ib(u+s)\psi'_{-1}(s) + c(u+s) \\ &\quad -a(u)\xi^2 - b(u)\xi - c(u). \end{aligned}$$

Assuming ellipticity, that is $a(x) \neq 0$ for all $x \in \mathbf{R}$, the eikonal identity $\phi_0 = 0$ implies

$$\psi_{-1}(s) = i \int_{v=0}^{s} \left\{ -\frac{b(u+v)}{2a(u+v)} + \sqrt{w(u,\xi,v)} \right\} \mathrm{d}v,$$

where

$$w(u,\xi,v) = \frac{a(u)\xi^2}{a(u+v)} + \frac{b(u)\xi}{a(u+v)} + \frac{b(u+v)^2}{4a(u+v)^2} + \frac{c(u) - c(u+v)}{a(u+v)}.$$

We take the branch of the square root which equals $\xi + b(u)/2a(u)$ at $v = 0$. Condition (24) implies that $\partial\sigma/\partial\xi \neq 0$ and hence that $w(u,\xi,0)$ is non-zero; this implies that $w(u,\xi,v) \neq 0$ for all small enough v; and hence that the square root is uniquely determined for all such v by the requirement of continuity.

Writing $\psi_{-1}(s) = i\xi s + ks^2/2 + O(s^3)$ for some $k \in \mathbf{C}$, we then obtain

$$-\mathrm{i}k\{2a(u)\xi + b(u)\} + a'(u)\xi^2 + b'(u)\xi + c'(u) = 0.$$

The requirement that $\mathrm{Re}(k) < 0$ may be rewritten in the form

$$\mathrm{Im}\left(\frac{\partial\sigma}{\partial u} \frac{\partial\overline{\sigma}}{\partial\xi} \right) < 0$$

and then in the form $(u, \xi) \in \Omega$ where

$$\Omega = \{(u,\xi) : \{\sigma_1, \sigma_2\} > 0\} \tag{24}$$

and

$$\{\sigma_1, \sigma_2\} := \frac{\partial\sigma_1}{\partial u}\frac{\partial\sigma_2}{\partial\xi} - \frac{\partial\sigma_1}{\partial\xi}\frac{\partial\sigma_2}{\partial u}$$

and $\sigma_1 = \mathrm{Re}(\sigma)$, $\sigma_2 = \mathrm{Im}(\sigma)$. In examples one may find that Ω is not connected. If it has components Λ_j then $\sigma(\Omega_j)$ may overlap. The multiplicity of a point $z \in \sigma(\Omega)$ may be defined by

$$m_L(z) = \#\{(u, \xi) \in \Omega : \sigma(u, \xi) = z\}.$$

If the coefficients of L_h are smooth then for any choice of n one may choose $\psi_0, \ldots, \psi_n$ so that $\phi_1 = \cdots = \phi_{n+1} = 0$. This is achieved as follows. If $1 \leqslant m \leqslant n$ then

$$\phi_{m+1} = (-2a\psi'_{-1} - ib)\psi'_m + F_m(\psi_{-1}, \ldots, \psi_{m-1}).$$

It follows from (24) that $2a\psi'_{-1} + ib \neq 0$ if $s = 0$, and hence that it is non-zero for all small enough s. If we define ψ_m by

$$\psi_m(s) = \int_0^s \frac{F_m(\psi_{-1}, \ldots, \psi_{m-1})}{2a\psi'_{-1} + ib}\, \mathrm{d}v.$$

Then $|\psi_m(s)| \leqslant c_m|s|$ and $\phi_{m+1}(s) = 0$ for all small enough s. On making these choices we obtain a pseudo-eigenfunction f, depending on h, n, u and ξ, for which $L_h f - \sigma(u, \xi) f = O(h^{n+2})$ as $h \to 0$.

The proof of Theorem 13 below is facilitated by introducing the scale of spaces $\mathscr{E}^\gamma$, consisting of all functions which can be written as finite sums of functions of the form $g(s) = h^{\alpha - 1/4} s^\beta \rho(s) \exp\{\psi(s)\}$ where ψ is given by (22), $\rho \in C^\infty$ has support in $[-\delta, \delta]$, $\alpha \in \mathbf{R}$, $\beta \in \{0, 1, 2, \ldots\}$ and $2\alpha + \beta \geqslant \gamma$. Putting $\mathscr{E}^\infty = \cap_{\gamma \in \mathbf{R}} \mathscr{E}^\gamma$ we see that if, in addition to the above assumptions, ρ vanishes in some neighbourhood of 0, then $g \in \mathscr{E}^\infty$.

Lemma 12. *If $\delta > 0$ is small enough and $g \in \mathscr{E}^\gamma$ then there exists c such that*

$$\|g\| \leqslant c h^{\gamma/2}$$

for all $0 < h \leqslant 1$.

Proof. It is sufficient to consider the case in which g is one of the terms of the form assumed in the definition of $\mathscr{E}^\gamma$. One may rewrite $|h^{1/4-\alpha} g(s)|^2$ in the form $s^{2\beta} G(s) \exp\{-h^{-1} s^2 F(s)\}$ where $F(s) = -2\,\mathrm{Re}(\psi_{-1}(s)/s^2)$ is a positive continuous function on $[-\delta, \delta]$ if $\delta > 0$ is small enough and G is a continuous function on $[-\delta, \delta]$. By Laplace's method we have

$$\int_{-\delta}^{\delta} s^{2\beta} G(s) \exp\left\{-h^{-1} s^2 F(s)\right\} \mathrm{d}s \sim c h^{(2\beta+1)/2}$$

as $h \to 0+$, where

$$c = \frac{G(0)\Gamma((2\beta+1)/2)}{F(0)^{(2\beta+1)/2}}.$$

The statement of the lemma follows immediately. □

Theorem 13. *If the coefficients of L_h are C^∞ and (u,ξ) lies in the set Ω defined by* (24), *then for every positive integer n there exist functions $f \in C_c^\infty$ depending on h, n, u, ξ such that*

$$\lim_{h\to 0} \|f\| = c > 0, \tag{25}$$

$$\|Qf - uf\| = O(h^{1/2}), \tag{26}$$

$$\|Pf - \xi f\| = O(h^{1/2}), \tag{27}$$

$$\|L_h f - \sigma(u,\xi) f\| = O(h^{n+2}) \tag{28}$$

as $h \to 0$.

Proof. We define f by (21) and observe that $f \in \mathscr{E}^0$. The asymptotic formula (25) follows by the method of proof of Lemma 12. We next observe that $Qf - uf \in \mathscr{E}^1$ so (26) follows from Lemma 12.

We have

$$Pf - \xi f = \mu_1 + \mu_2 + \mu_3,$$

where

$$\mu_1 = -ih^{-1/4}\{\psi'_{-1}(s) - i\xi\}\chi(s)\exp\{\psi(s)\} \in \mathscr{E}^1,$$

$$\mu_2 = -ih^{3/4}\left\{\sum_{m=0}^{n} h^m \psi'_m(s)\right\}\chi(s)\exp\{\psi(s)\} \in \mathscr{E}^2,$$

$$\mu_3 = -ih^{3/4}\chi'(s)\exp\{\psi(s)\} \in \mathscr{E}^\infty.$$

Therefore, $Pf - \xi f \in \mathscr{E}^1$ and (27) follows using Lemma 12.

Since $\phi_m = 0$ for $0 \leqslant m \leqslant n+1$ it follows from (23) that

$$L_h f - \sigma(u,\xi) f = \left(\sum_{m=n+2}^{2n+2} h^m \phi_m\right) f + O(h^\infty)$$

$$\in \mathscr{E}^{2n+4}.$$

This implies (28) by Lemma 12. □

Note: The orders of magnitude of the errors in *both* (26) and (27) cannot be reduced by a different choice of the function f, because of the uncertainty principle.

The following lemma shows that one can approximate the pseudo-eigenfunction by a Gaussian expression.

Lemma 14. *We have*

$$\|f-g\| \leqslant ch^{1/2}$$

as $h \to 0$, *where*

$$g(u+s) = h^{-1/4}\exp\{h^{-1}(i\xi s + ks^2/2)\}.$$

Proof. Since $g - \chi g = O(h^\infty)$ we have to estimate the L^2 norm of

$$h^{-1/4}\chi(s)\left(\exp\left\{\psi(s)\right\} - \exp\{h^{-1}(i\xi s + ks^2/2)\right\}\right).$$

By virtue of the bound

$$|\mathrm{e}^{-a} - \mathrm{e}^{-b}| \leqslant |a-b|\mathrm{e}^{-\min(\mathrm{Re}(a),\mathrm{Re}(b))}$$

this is dominated by the absolute value of

$$\mu(s) = h^{-1/4}\left\{\psi(s) - h^{-1}(i\xi s + ks^2/2)\right\}\chi(s)\exp\left\{-h^{-1}cs^2\right\}$$

for some $c > 0$. In the following calculations we define $\tilde{\mathscr{E}}^\gamma$ in the same way as $\mathscr{E}^\gamma$ but with $\psi(s)$ replaced by $-h^{-1}cs^2$. We may write $\mu = \mu_1 + \mu_2$ where

$$\begin{aligned}\mu_1(s) &= h^{-1/4}\left\{\psi_{-1}(s) - h^{-1}(i\xi s + ks^2/2)\right\}\chi(s)\exp\left\{-h^{-1}cs^2\right\},\\ \mu_2(s) &= h^{-1/4}\left(\sum_{m=0}^{n} h^m\psi_m(s)\right)\chi(s)\exp\left\{-h^{-1}cs^2\right\}.\end{aligned}$$

Since

$$|\psi_{-1}(s) - h^{-1}(i\xi s + ks^2/2)| \leqslant c_{-1}h^{-1}|s|^3$$

we have $\mu_1 \in \tilde{\mathscr{E}}^1$. Since $|\psi_m(s)| \leqslant c_m|s|$ for all s we also have $\mu_2 \in \tilde{\mathscr{E}}^1$. The estimate of this lemma now follows by an obvious modification of Lemma 12. $\square$

8. A semi-classical transform

We continue with the assumptions and notation of the last section. Theorem 13 provides the information needed for the application of Theorem 6. We define the set Ω in Theorem 6 by (24) and take σ to be the semi-classical principal symbol (15) of A. In numerical applications, one would, of course, have to restrict to a finite subset of Ω, as described in [6].

We fix n and put $e_{h,u,\xi} = f_{h,u,\xi}/\|f_{h,u,\xi}\|$ where $f_{h,u,\xi} = f$ is defined by (21). The semi-classical integral transform $E : L^1(\Omega) \to L^2(\mathbf{R})$ is then defined by

$$(E_h\phi)(x) = \int_\Omega \phi(u,\xi)e_{h,u,\xi}(x)\,\mathrm{d}u\,\mathrm{d}\xi$$

and has norm 1 by [10, Theorem VI.8.6]. The functions $f_{h,u,\xi}(x)$ are very complicated for large n, and the following approximation may therefore be valuable.

Theorem 15. *Given h, u, ξ, let*

$$g_{h,u,\xi}(x) = h^{-1/4}\exp\left\{h^{-1}(i\xi(x-u) + k_{u,\xi}(x-u)^2/2)\right\}, \tag{29}$$

where

$$k_{u,\xi} = -i\frac{\partial\sigma}{\partial u}\left\{\frac{\partial\sigma}{\partial\xi}\right\}^{-1}. \tag{30}$$

If $(u,\xi) \in \Omega$ then $g_{h,u,\xi} \in L^2(\mathbf{R})$. Define $E'_h : L^1(\Omega) \to L^2(\mathbf{R})$ by

$$(E'_h\phi)(x) = \int_\Omega \phi(u,\xi)e'_{h,u,\xi}(x)\,\mathrm{d}u\,\mathrm{d}\xi, \tag{31}$$

where $e'_{h,u,\xi} = g_{h,u,\xi}/\|g_{h,u,\xi}\|$. Then $\|E'_h\| = 1$ and

$$\lim_{h\to 0}\|E_h\phi - E'_h\phi\| = 0 \tag{32}$$

for all $\phi \in L^1(\Omega)$. If we replace Ω by a compact subset U of Ω then

$$\lim_{h\to 0}\|E_h - E'_h\| = 0. \tag{33}$$

Proof. We start by observing that $\mathrm{Re}(k_{u,\xi}) < 0$ if and only if $(u,\xi) \in \Omega$, so $g_{h,u,\xi} \in L^2(\mathbf{R})$ under the same conditions. We have $\|E'_h\| = 1$ by [10, Theorem VI.8.6].

Let $\{\Omega_n\}_{n=1}^{\infty}$ be an increasing sequence of compact subsets of Ω whose union equals Ω. If we can prove that the restrictions $E_{h,n}$ and $E'_{h,n}$ to $L^1(\Omega_n)$ satisfy

$$\lim_{h\to 0} \|E_{h,n} - E'_{h,n}\| = 0 \tag{34}$$

then (32) and (33) follow by standard procedures.

In Lemma 14 we proved that

$$\|f_{h,u,\xi} - g_{h,u,\xi}\| = O(h^{1/2})$$

for each $(u,\xi) \in \Omega$ as $h \to 0$. The dependence of the error upon u, ξ and the coefficients of A was given explicitly, and implies that

$$\lim_{h\to 0} \sup\{\|f_{h,u,\xi} - g_{h,u,\xi}\| : (u,\xi) \in \Omega_n\} = 0.$$

Taking (25) into account we deduce that

$$\lim_{h\to 0} \sup\left\{\|e_{h,u,\xi} - e'_{h,u,\xi}\| : (u,\xi) \in \Omega_n\right\} = 0.$$

This implies (34). $\square$

Lemma 16. *Let $E'_{h,U}$ denote the restriction of E'_h to the subset U of Ω. If U, V are two compact subsets of Ω which are spatially disjoint in the sense that $(u,\xi) \in U$ and $(v,\eta) \in V$ implies $u \neq v$ then the ranges of $E'_{h,U}$ and $E'_{h,V}$ are uniformly asymptotically orthogonal in the sense that*

$$\lim_{h\to 0} \|(E'_{h,U})^* E'_{h,V}\| = 0.$$

The convergence is exponentially fast.

Proof. Let W be an open subset of $\mathbf{R}$ such that $U \subseteq (W \times \mathbf{R})$ and $V \cap (\overline{W} \times \mathbf{R}) = \emptyset$. Let P be the orthogonal projection in $L^2(\mathbf{R})$ whose range consists of all functions with support in W. Then

$$\begin{aligned}\|(E'_{h,U})^* E'_{h,V}\| &\leqslant \|(E'_{h,U})^*(I-P)E'_{h,V}\| + \|(E'_{h,U})^* P E'_{h,V}\| \\ &\leqslant \|(I-P)E'_{h,U}\| + \|PE'_{h,V}\|.\end{aligned}$$

We consider further only the first term on the RHS; the other is treated in a similar manner. If $\phi \in L^1(U)$ then

$$\begin{aligned}\|(I-P)E'_h\phi\| &= \left\| \int_U (I-P)e'_{h,u,\xi}\phi(u,\xi)\,\mathrm{d}u\,\mathrm{d}\xi \right\| \\ &\leqslant \int_U \|(I-P)e'_{h,u,\xi}\|\,|\phi(u,\xi)|\,\mathrm{d}u\,\mathrm{d}\xi \\ &\leqslant \sup\left\{\|(I-P)e'_{h,u,\xi}\| : (u,\xi)\in U\right\}\,\|\phi\| \\ &\leqslant \frac{\sup\left\{\|(I-P)g_{h,u,\xi}\| : (u,\xi)\in U\right\}}{\inf\{\|g_{h,u,\xi}\| : (u,\xi)\in U\}}\|\phi\|.\end{aligned}$$

The explicit expression (29) for g and the compactness of U ensure that the final supremum converges to 0 exponentially fast as $h \to 0$ while the final infimum converges to a positive limit. □

If we subdivide $\mathbf{R}$ into small intervals then the lemma implies that E'_h (or more exactly its restriction to any compact subregion of Ω) acts asymptotically independently on subintervals which are not adjacent. If each interval is small enough we may approximate E'_h in any subinterval by the operator with a frozen value of u.

We conjecture that under suitable conditions on the coefficients of A, both the transforms E_h and E'_h are bounded from $L^2(\Omega)$ to $L^2(\mathbf{R})$. As evidence for this we treat the case in which the variable u in $k_{u,\xi}$ is frozen at the value v. We also assume that A is a Schrödinger operator, so that its symbol is of the form $\sigma(u,\xi) = \xi^2 + c(u)$. This implies that $k_{v,\xi} = -1/\kappa\xi$ where $\kappa = 2/ic'(v)$. Assuming that κ has positive real part, it is immediate that $\mathrm{Re}\,k_{v,\xi} < 0$ if and only if $\xi > 0$. We therefore put $\mathbf{R}^2_+ = \{(u,\xi) : u \in \mathbf{R}, \xi > 0\}$.

We define the distorted FBI transform $\tilde{E}_h : C_c(\mathbf{R}^2_+) \to L^2(\mathbf{R})$ by

$$\tilde{E}_h\phi = h^{-1/2}\int_{\mathbf{R}^2_+} \phi(u,\xi)\tilde{e}_{h,u,\xi}\,\mathrm{d}u\,\mathrm{d}\xi, \tag{35}$$

where $\tilde{e}_{h,u,\xi} = \tilde{g}_{h,u,\xi}/\|\tilde{g}_{h,u,\xi}\|$ and

$$\tilde{g}_{h,u,\xi}(x) = \exp\left\{i\xi(x-u)/h - (x-u)^2/2h\kappa\xi\right\}. \tag{36}$$

Theorem 17. *If* $\mathrm{Re}(\kappa) > 0$ *and* $h > 0$ *then operator* (35) *may be extended to a bounded operator from* $L^2(\mathbf{R}^2_+)$ *to* $L^2(\mathbf{R})$ *whose norm is bounded above uniformly as* $h \to 0$.

Proof. In this proof we write c_r to denote positive constants which depend only on κ. We always take ξ to be positive. We have

$$\begin{aligned}\|\tilde{g}_{h,u,\xi}\|^2 &= \int_{\mathbf{R}} \exp\left\{-\mathrm{Re}(1/\kappa)(x-u)^2/h\xi\right\} \mathrm{d}x \\ &= c_1 h^{1/2}\xi^{1/2}.\end{aligned}$$

Therefore,

$$\|\tilde{g}_{h,u,\xi}\| = c_2 h^{1/4}\xi^{1/4}.$$

We prove the L^2 boundedness of $\tilde{E}_h^*$ rather than that of $\tilde{E}_h$. We have

$$(\tilde{E}_h^* f)(u,\xi) = \int_{\mathbf{R}} K(u,\xi,h,x) f(x)\,\mathrm{d}x, \tag{37}$$

where

$$\begin{aligned}K(u,\xi,h,x) &= h^{-1/2}\overline{\tilde{e}_{h,u,\xi}(x)} = \beta_{h,\xi}\gamma_\xi(u-x),\\ \beta_{h,\xi} &= c_3 h^{-3/4}\xi^{-1/4},\\ \gamma_\xi(u) &= \exp\{i\xi u/h - u^2/2h\overline{\kappa}\xi\}.\end{aligned}$$

We next take the Fourier transform $\mathscr{F}$ of (37) in the u variable, noting that $\mathscr{F}$ is a unitary operator on $L^2(\mathbf{R}_+^2)$. This yields

$$\|\tilde{E}_h^* f\| = \|k\|,$$

where

$$k(s,\xi) = \beta_{h,\xi}\hat{\gamma}_\xi(s)(\mathscr{F} f)(s)$$

and

$$\begin{aligned}\hat{\gamma}_\xi(s) &= \int_{\mathbf{R}} \exp\{iu(\xi/h - s) - u^2/2h\overline{\kappa}\xi\}\,\mathrm{d}u\\ &= c_4 h^{1/2}\xi^{1/2}\exp\left\{-(\xi/h - s)^2 h\overline{\kappa}\xi/2\right\}.\end{aligned}$$

We deduce that

$$\|\tilde{E}_h^* f\| \leqslant c_5\|\mathscr{F} f\| = c_5\|f\|$$

for all $f \in L^2(\mathbf{R})$ if and only if

$$\sup_{s\in\mathbf{R}} \left\{ \int_0^\infty \left|\beta_{h,\xi}\hat{\gamma}_\xi(s)\right|^2 \, \mathrm{d}\xi \right\} \leqslant c_5^2.$$

Our task therefore, is to prove that the function

$$F(h,s) = \int_0^\infty h^{-1/2}\xi^{1/2} \exp\left\{-c_6(\xi/h - s)^2 h\xi\right\} \mathrm{d}\xi \tag{38}$$

is bounded on $\mathbf{R}^+ \times \mathbf{R}$, provided $c_6 > 0$. If $s \leqslant 0$ then putting $\xi = h^{1/3}\eta$ we obtain

$$\begin{aligned} F(h,s) &\leqslant F(h,0) \\ &= \int_0^\infty h^{-1/2}\xi^{1/2} \exp\left\{-c_6\xi^3/h\right\} \mathrm{d}\xi \\ &= \int_0^\infty \eta^{1/2} \exp\left\{-c_6\eta^3\right\} \mathrm{d}\eta, \end{aligned}$$

which is finite. If $s > 0$ then putting $\xi = hs\eta$ we obtain

$$F(h,s) = G(h^2 s^3), \tag{39}$$

where

$$G(t) = \int_0^\infty \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t} \, \mathrm{d}\eta,$$

so we have to prove that G is bounded on $(0,\infty)$. We do this in stages. If $0 \leqslant t \leqslant 1$ then

$$\int_0^{1/2} \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t} \, \mathrm{d}\eta \leqslant 1/2$$

because every term in the integrand is less than 1. If $t \geqslant 1$ then

$$\begin{aligned} \int_0^{1/2} \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t} \, \mathrm{d}\eta &\leqslant \int_0^{1/2} \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6\eta t/4} \, \mathrm{d}\eta \\ &\leqslant \int_0^\infty \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6\eta t/4} \, \mathrm{d}\eta \\ &= c_7 t^{-1} \leqslant c_7. \end{aligned}$$

If $t > 0$ then

$$\begin{aligned}\int_{1/2}^{4} \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t}\,\mathrm{d}\eta &\leqslant \int_{1/2}^{4} 2t^{1/2}\mathrm{e}^{-c_6(\eta-1)^2 t/2}\,\mathrm{d}\eta\\ &\leqslant \int_{-\infty}^{\infty} 2t^{1/2}\mathrm{e}^{-c_6\eta^2 t/2}\,\mathrm{d}\eta\\ &= c_8.\end{aligned}$$

Finally, if $t > 0$ then putting $\eta = \zeta t^{-1/3}$ we obtain

$$\begin{aligned}\int_{4}^{\infty} \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t}\,\mathrm{d}\eta &\leqslant \int_{4}^{\infty} \eta^{1/2} t^{1/2}\mathrm{e}^{-c_8\eta^3 t}\,\mathrm{d}\eta\\ &\leqslant \int_{0}^{\infty} \zeta^{1/2}\mathrm{e}^{-c_8\zeta^3}\,\mathrm{d}\zeta\\ &= c_9. \quad \square\end{aligned}$$

One cannot expect E_h^* to be isometric, as is the case for the FBI transform, but we prove that this is asymptotically true in the semi-classical limit, up to a normalizing constant c, which could be evaluated explicitly.

Theorem 18. *There exists a positive constant c such that*

$$\lim_{h\to 0} \|E_h^* f\| = c\|f\|$$

for all $f \in L^2(\mathbf{R})$.

Proof. In the proof of Theorem 17 we obtained the formula

$$\|E_h^* f\|^2 = c_{10}\int_{-\infty}^{\infty} F(h,s)|(\mathscr{F} f)(s)|^2\,\mathrm{d}s,$$

where

$$0 \leqslant F(h,s) \leqslant c_{11}$$

for all $h > 0$ and $s \in \mathbf{R}$. By the dominated convergence theorem it suffices to prove that

$$\lim_{h\to 0} F(h,s) = c_{12} := \int_0^{\infty} \eta^{1/2} \exp\left\{-c_6\eta^3\right\}\,\mathrm{d}\eta$$

for all $s \in \mathbf{R}$. We do this for $s > 0$, noting that the cases $s = 0$ and $s < 0$ are similar. By (39) it suffices to prove that $\lim_{t\to 0+} G(t) = c_{12}$. As $t \to 0+$ we have

$$\begin{aligned} G(t) &= \int_0^\infty \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6(\eta-1)^2\eta t}\,\mathrm{d}\eta \\ &\sim \int_0^\infty \eta^{1/2} t^{1/2} \mathrm{e}^{-c_6\eta^3 t}\,\mathrm{d}\eta \\ &= c_{12} \end{aligned}$$

using the change of variable $\eta \to \eta t^{-1/3}$. □

In order to extend Theorem 17 to second-order differential operators other than Schrödinger operators, it needs to be generalized as follows.

Theorem 19. *Let* $\kappa : (0, \infty) \to \mathbf{C}$ *be a continuous function, let* c_0, c_∞ *be positive constants and let* α_0, α_∞ *be non-negative constants such that*

$$\begin{aligned} c_0^{-1}\xi^{\alpha_0} &\leqslant \operatorname{Re}\kappa(\xi) \leqslant c_0\xi^{\alpha_0} \quad \text{if } 0 < \xi \leqslant 1, \\ c_\infty^{-1}\xi^{\alpha_\infty} &\leqslant \operatorname{Re}\kappa(\xi) \leqslant c_\infty\xi^{\alpha_\infty} \quad \text{if } 1 \leqslant \xi < \infty. \end{aligned}$$

Then the conclusion of Theorem 17 *is still valid if we replace* (36) *by*

$$\tilde{g}_{h,u,\xi}(x) = \exp\left\{ i\xi(x-u)/h - (x-u)^2/2h\kappa(\xi) \right\}.$$

Proof. We make obvious adaptations to the proof of Theorem 17 up to (38), which becomes

$$\begin{aligned} F(h,s) &= \int_0^\infty h^{-1/2} (\operatorname{Re}\kappa(\xi))^{1/2} \exp\left\{ -c_6(\xi/h - s)^2 h \operatorname{Re}\kappa(\xi) \right\} \mathrm{d}\xi \\ &\leqslant \int_0^1 h^{-1/2} c_0^{1/2} \xi^{\alpha_0/2} \exp\left\{ -c_6(\xi/h - s)^2 h c_0^{-1} \xi^{\alpha_0} \right\} \mathrm{d}\xi \\ &\quad + \int_1^\infty h^{-1/2} c_\infty^{1/2} \xi^{\alpha_\infty/2} \exp\left\{ -c_6(\xi/h - s)^2 h c_\infty^{-1} \xi^{\alpha_\infty} \right\} \mathrm{d}\xi. \end{aligned}$$

Each of these integrals is estimated by the same method as in Theorem 17. □

9. Constructing the boundary pseudo-spectra

When one examines the pseudo-eigenfunctions in several exactly soluble examples, [5,6,18,19], one sees that they do not conform to the above ideas. They are strongly localized at one end of the interval in question, and decrease exponentially as one moves away from this end.

In this section, we develop the general theory of boundary pseudo-spectra for variable coefficient operators in the one-dimensional context. A partial extension to higher dimensions and manifolds is described in the next section. We assume that

$$(L_h f)(x) = -h^2 a(x) f''(x) - ihb(x) f'(x) + c(x) f(x)$$

for $x \in [0, \gamma]$. The semi-classical principal symbol is

$$\sigma(u, \xi) = a(u)\xi^2 + b(u)\xi + c(u).$$

We will need the fact that the symbol can be analytically continued to complex ξ, but only assume the coefficients of L_h, and therefore σ, to be C^∞ in u on $[0, \gamma]$. Similar but weaker estimates can be proved if the coefficients are only C^n for some n. We assume ellipticity, in other words that $a(x) \neq 0$ for all $x \in [0, \gamma]$. We start by ignoring the boundary conditions and looking for a pseudo-eigenfunction of the form

$$f(s) = h^{-1/2} \chi(s) \exp(\psi(s)), \tag{40}$$

where

$$\psi(s) = \sum_{m=-1}^{n} h^m \psi_m(s).$$

We assume that $\chi \in C^\infty[0, \gamma]$ satisfies $\chi(s) = 1$ if $0 \leqslant s \leqslant \delta/2$ and $\chi(s) = 0$ if $s \geqslant \delta$; the constant $\delta > 0$ must be small enough for the proof of Theorem 21 to be valid. We put

$$\psi_{-1}(s) = i \int_{v=0}^{s} \left\{ -\frac{b(v)}{2a(v)} + \sqrt{w(\xi, v)} \right\} \mathrm{d}v,$$

where

$$w(\xi, v) = \frac{a(0)\xi^2}{a(v)} + \frac{b(0)\xi}{a(v)} + \frac{b(v)^2}{4a(v)^2} + \frac{c(0) - c(v)}{a(v)}.$$

As before we take the branch of the square root which equals $\xi + b(0)/2a(0)$ at $v = 0$. However we now require $\mathrm{Im}(\xi) > 0$, in order to ensure that $f(s)$ decays rapidly as s increases. We have

$$\psi_{-1}(s) = i\xi s + ks^2/2 + O(s^3)$$

for small $s > 0$ as before.

Lemma 20. *Let F be a positive continuous function on $[0, \delta]$ and let G be a continuous function on $[0, \delta]$. If m is a non-negative even integer then*

$$\int_0^\delta s^m G(s) \exp\left\{-h^{-1} s F(s)\right\} \mathrm{d}s \sim c h^{m+1}$$

as $h \to 0+$, where

$$c = \frac{G(0)\Gamma(m+1)}{F(0)^{m+1}}.$$

In the following theorem we put $(Qf)(x) = xf(x)$ and $(Pf)(x) = -ihf'(x)$ as before. Although Q is self-adjoint on an obvious domain, we impose no boundary conditions on P, which is therefore not even symmetric.

Theorem 21. *If the coefficients of L_h are C^∞ and $\mathrm{Im}(\xi) > 0$ then for any positive integer n there exist functions f which depend on h, n, ξ such that*

$$\lim_{h \to 0} \|f\| = c > 0, \tag{41}$$

$$\|Qf\| = O(h), \tag{42}$$

$$\|Pf - \xi f\| = O(h), \tag{43}$$

$$\|L_h f - \sigma(0, \xi) f\| = O(h^{n+2}) \tag{44}$$

as $h \to 0$.

Proof. Let f be given by (40). To prove (41) we write

$$\begin{aligned} \|f\|^2 &= h^{-1} \int_0^\delta \chi(s)^2 \exp\{2\,\mathrm{Re}(\psi(s))\}\,\mathrm{d}s \\ &= h^{-1} \int_0^\delta G(s) \exp\{-h^{-1} s F(s)\}\,\mathrm{d}s, \end{aligned}$$

where

$$\begin{aligned} F(s) &= -2\,\mathrm{Re}(\psi_{-1}(s))/s, \\ G(s) &= \chi(s)^2 \exp\left\{2\,\mathrm{Re}\left(\sum_{m=0}^{n} h^m \psi_m(s)\right)\right\}. \end{aligned}$$

This is of the form treated by Lemma 20 if $\delta > 0$ is small enough to ensure that $F(s) > 0$ for all $s \in [0, \delta]$.

To prove (42) we write

$$\|Qf\|^2 = h^{-1} \int_0^{\delta} s^2 G(s) \exp\left\{ -h^{-1} s F(s) \right\} \mathrm{d}s$$

and apply Lemma 20 again.

The proof of (43) uses Lemma 20 and the expansion

$$Pf - \xi f = \mu_1 + \mu_2 + \mu_3,$$

where

$$\begin{aligned}
\mu_1 &= -ih^{-1/2}\{\psi'_{-1}(s) - i\xi)\}\chi(s)\exp\{\psi(s)\},\\
\mu_2 &= -ih^{1/2}\left(\sum_{m=0}^{n} h^m \psi'_m(s)\right)\chi(s)\exp\{\psi(s)\},\\
\mu_3 &= -ih^{1/2}\chi'(s)\exp\{\psi(s)\}.
\end{aligned}$$

The proof of (44) follows in a similar way from the formula

$$L_h f - \sigma(0,\xi) f = \left(\sum_{m=n+2}^{2n+2} h^m \phi_m\right) f + O(h^\infty). \qquad \square$$

We finally assume the boundary conditions

$$uhf'(0) + wf(0) = 0 \tag{45}$$

for some complex constants u, w, both not zero. We say that L_h satisfies the exit condition at 0 if $\mathrm{Im}(-b(0)/a(0)) > 0$. This language is motivated by the example discussed in [6], in which L_h is the generator of a subMarkov diffusion on an interval. Given the exit condition at 0, we define the boundary semi-classical pseudo-spectrum at 0 to be the set

$$\tilde{\Lambda} = \{\xi : 0 < \mathrm{Im}(\xi) < \mathrm{Im}(-b(0)/a(0))\}. \tag{46}$$

If $\xi_1 \in \tilde{\Lambda}$ and $z = \sigma(0,\xi_1)$ then the other solution ξ_2 of $\sigma(0,\xi) = z$ also lies in $\tilde{\Lambda}$. We have $\xi_1 = \xi_2$ if and only if $z = c(0) - b(0)^2/4a(0)$. The set $\sigma(0,\tilde{\Lambda})$ is the region inside the parabola $P = \{\sigma(0,t) : t \in \mathbf{R}\}$.

Those familiar with [5,18,19] will observe the close relationship between the above and the winding number calculations there. At a qualitative level the given operator can be approximated near the end of the interval by the operator whose coefficients are frozen to the values which they have at the endpoint. Our theorem below provides quantitative flesh to this idea. It also provides the precise form of the relevant pseudo-eigenfunction, which is not easy to guess from the constant coefficient case.

Theorem 22. *Let L_h satisfy the exit condition at* 0 *and let z lie inside the parabola P. Assuming $z \neq c(0) - b(0)^2/4a(0)$, let $\xi_1,\ \xi_2 \in \tilde{\Lambda}$ denote the two distinct solutions of $\sigma(0, \xi) = z$. Given $h > 0$ and $n \geqslant 1$, let f_r be the boundary pseudo-eigenfunctions associated with h, n, ξ_r as in* (40) *and Theorem* 21, *and let*

$$f = (iu\xi_2 + w)f_1 - (iu\xi_1 + w)f_2. \tag{47}$$

Then f satisfies the boundary condition (45) *at* 0 *and*

$$\|L_h f - zf\|/\|f\| = O(h^{n+2}) \tag{48}$$

as $h \to 0$.

Proof. The assumptions imply that f_r satisfy the estimates of Theorem 21, from which (48) follows. The proof that f satisfies (45) depends upon the identities $f_r(0) = h^{-1/2}$ and $f_r'(0) = ih^{-3/2}\xi_r$. $\square$

10. Higher dimensions

The extension of the above ideas to higher dimensions needs more machinery. We are mainly interested in bounded regions in $\mathbf{R}^N$ with smooth boundary, but since the proof of our main result depends upon choosing local coordinates around a boundary point rather carefully, we write down the argument in a manifold context. Let X be a smooth N-dimensional manifold with boundary ∂X. Let X be provided with a volume measure $\mathrm{d}vol$ which has positive C^∞ density $v(x)$ when restricted to any coordinate neighbourhood U.

The natural differential $\mathrm{d} : C^n(X) \to C^{n-1}(T^*X)$ is given within U by

$$\mathrm{d}f(x) = (\partial_1 f(x), \ldots, \partial_n f(x))$$

and the adjoint operator $\mathrm{d}^* : C^n(TX) \to C^{n-1}(X)$ acts on a section $g \in C^n(TU)$ by

$$\mathrm{d}^* g(x) = -v(x)^{-1}\partial_j(v(x)g^j(x)).$$

The differential operator L_h is determined by three coefficient functions, all assumed to be C^∞ and complex-valued on X; we write T_x and T_x^* in place of $T_x \otimes \mathbf{C}$ and $T_x^* \otimes \mathbf{C}$ below. We assume that $a(x) : T_x^* \to T_x$, $b(x) \in T_x$ and $c(x) \in \mathbf{C}$ for all $x \in X$.

Given $h>0$ and $f\in C^\infty(X)$ we then put

$$(L_h f)(x)=h^2\,\mathrm{d}^*(a(x)\,\mathrm{d}f(x))-ihb(x)\cdot\mathrm{d}f(x)+c(x)f(x).$$

Throughout this section a dot indicates the natural action of a covector on a tangent vector at some point of X. In the coordinate neighbourhood U the above formula may be written in the form

$$(L_h f)(x)=-h^2v^{-1}(x)\partial_j\left(v(x)a^{j,k}(x)\partial_k f(x)\right)-ihb^j(x)\partial_j f(x)+c(x)f(x)$$

using the usual summation convention, or in the form

$$(L_h f)(x)=-h^2a^{j,k}(x)\partial_{j,k}f(x)-ihb^j(h,x)\partial_j f(x)+c(h,x)f(x), \tag{49}$$

where

$$b^j(h,x)\;=\;b^j(x)+hb_1^j(x), \tag{50}$$

$$c(h,x)\;=\;c(x)+hc_1(x)+h^2c_2(x). \tag{51}$$

The set of all operators of form (49) is invariant under changes of local coordinates.

The symbol of L_h is given by

$$\sigma_h(x,\xi)=h^2a^{j,k}(x)\xi_j\xi_k+hb^j(h,x)\xi_j+c(h,x)$$

which is not an invariant expression: both d^* and L_h depend upon the choice of the density v. However the semi-classical principal symbol

$$\begin{aligned}\sigma(x,\xi)\;&=\;\lim_{h\to 0}\,\sigma_h(x,h^{-1}\xi)\\&=\;a^{j,k}(x)\xi_j\xi_k+b^j(x)\xi_j+c(x)\\&=\;a(x)\xi\cdot\xi+b(x)\cdot\xi+c(x)\end{aligned}$$

is invariant under changes of local coordinates.

The following theorem is a multi-dimensional ‘boundary’ analogue of Theorem 11. We expect that there is also a multi-dimensional analogue of Theorem 22. We choose a point in ∂X, label it p, and choose a complex cotangent vector ξ at p. We require that $\mathrm{Im}(\xi)$ has zero dot product with any vector at p which is tangent to ∂X and positive dot product with any inward pointing vector at p. If U is a coordinate neighbourhood around p we always assume that p is represented by the point $0\in\mathbf{R}^N$.

Theorem 23. *Let L_h be of form* (49) *where all of the coefficients in* (49), (50), (51) *are C^∞ functions on U. Let the complex cotangent vector ξ at $0 \in \partial X$ satisfy the conditions of the last paragraph. Then for every sufficiently small $h > 0$ there exists $f_h \in C^\infty(X)$ which vanishes outside a neighbourhood of* 0 *whose radius is of order $h^{1/2}$, and satisfies*

$$\lim_{h\to 0} \|f_h\|_2 = c > 0, \tag{52}$$

$$\|L_h f_h - \sigma(0,\xi) f_h\|_2 = O(h^{1/2}) \tag{53}$$

as $h \to 0$.

Proof. Let $\mathbf{R}_+^N$ denote the set of $x \in \mathbf{R}^N$ for which $x^N \geqslant 0$ and let $\mathbf{R}_0^N$ denote the set of x for which $x^N = 0$. We choose local coordinates around 0 such that

$$U = \left\{x \in \mathbf{R}_+^N : |x| < \rho\right\}$$

and put

$$\partial U = \left\{x \in \mathbf{R}_0^N : |x| < \rho\right\}$$

for some $\rho > 0$. We write $x = (x', x^N)$ where $x' \in \mathbf{R}^{N-1}$ and $x^N \in \mathbf{R}$. Our assumptions imply that $\xi = (\xi', \xi^N)$ where ξ' is real and $\eta := \mathrm{Im}(\xi^N) > 0$.

Put $\alpha = 1/2$ and $\gamma = (N+1)/4$. Let ϕ_1 be a smooth function on $\mathbf{R}^{N-1}$ which equals 1 if $|x'| \leqslant 1$ and 0 if $|x'| \geqslant 2$. Let ϕ_2 be a smooth function on $[0,\infty)$ which equals 1 if $0 \leqslant x^N \leqslant 1$ and 0 if $x^N \geqslant 2$. Let $\phi(x) = \phi_1(x')\phi_2(x^N)$. Then the smooth function

$$f_h(x) = h^{-\gamma} \mathrm{e}^{ih^{-1}\xi\cdot x} \phi(h^{-\alpha}x)$$

on U has support with the required property for all small enough $h > 0$.

To prove (52) we observe that

$$\begin{aligned} \|f_h\|_2^2 &\sim v(0)h^{-2\gamma} \int_{\mathbf{R}^{N-1}} \phi_1(h^{-\alpha}x')^2 \,\mathrm{d}^{N-1}x' \int_0^\infty \mathrm{e}^{-2h^{-1}\eta x^N} \phi_2(h^{-\alpha}x^N)^2 \,\mathrm{d}x^N \\ &= v(0)h^{-2\gamma+(N-1)\alpha+1} \int_{\mathbf{R}^{N-1}} \phi_1(y')^2 \,\mathrm{d}^{N-1}y' \int_0^\infty \mathrm{e}^{-2\eta s} \phi_2(h^{1-\alpha}s)^2 \,\mathrm{d}s \\ &\to v(0)(2\eta)^{-1} \int_{\mathbf{R}^{N-1}} \phi_1(y')^2 \,\mathrm{d}^{N-1}y' > 0 \end{aligned}$$

as $h \to 0$.

The proof of (53) depends upon writing

$$L_h f_h - \sigma(0,\xi) f_h = \sum_{m=1}^{7} g_m,$$

where

$$\begin{aligned}
g_1 &= h^{-\gamma}\left\{a^{j,k}(x) - a^{j,k}(0)\right\}\xi_j\xi_k \mathrm{e}^{ih^{-1}\xi\cdot x}\phi(h^{-\alpha}x),\\
g_2 &= -ih^{1-\alpha-\gamma}a^{j,k}(x)\xi_j \mathrm{e}^{ih^{-1}\xi\cdot x}\phi_k(h^{-\alpha}x),\\
g_3 &= -ih^{1-\alpha-\gamma}a^{j,k}(x)\xi_k \mathrm{e}^{ih^{-1}\xi\cdot x}\phi_j(h^{-\alpha}x),\\
g_4 &= -h^{2-2\alpha-\gamma}a^{j,k}(x)\mathrm{e}^{ih^{-1}\xi\cdot x}\phi_{j,k}(h^{-\alpha}x),\\
g_5 &= h^{-\gamma}\left\{b^j(h,x) - b^j(0)\right\}\xi_j \mathrm{e}^{ih^{-1}\xi\cdot x}\phi(h^{-\alpha}x),\\
g_6 &= -ih^{1-\alpha-\gamma}b^j(h,x)\mathrm{e}^{ih^{-1}\xi\cdot x}\phi_j(h^{-\alpha}x),\\
g_7 &= h^{-\gamma}\{c(h,x) - c(0)\}\mathrm{e}^{ih^{-1}\xi\cdot x}\phi(h^{-\alpha}x).
\end{aligned}$$

We estimate the L^2 norm of each of these as above, obtaining $\|g_r\|_2 = O(h^\alpha)$ for $r = 1, 5, 7$, $\|g_r\|_2 = O(h^{1-\alpha})$ for $r = 2, 3, 6$ and $\|g_r\|_2 = O(h^{2-2\alpha})$ for $r = 4$. Given these estimates, the optimal value of α is $1/2$. $\square$

We next impose boundary conditions of the form

$$hu(x')n(x',0)\cdot \mathrm{d}f(x',0) + w(x')f(x',0) = 0$$

for all $x' \in \partial U$, where the complex-valued coefficients u, w are C^∞ on ∂U; we assume non-degeneracy of the boundary conditions at 0 in the sense that both $u(0')$ and $w(0')$ do not vanish. The real vector field n on U is supposed to be smooth and transversal in the sense that it has a non-zero inward pointing component at every point of ∂U. We use the associated flow to construct local coordinates. In other words we choose local coordinates for which the boundary conditions can be written in the form

$$h\,u(x')\partial_N f(x',0) + w(x')f(x',0) = 0. \tag{54}$$

We say that the complex covector ξ at 0 is admissible under the following conditions. We require that $\mathrm{Im}(\xi)$ has positive dot product with any inward pointing vector at 0. We require that the same conditions hold for a second complex covector $\tilde{\xi}$ at 0. We require that $z := \sigma(0,\xi) = \sigma(0,\tilde{\xi})$ and that $\xi\cdot t = \tilde{\xi}\cdot t \in \mathbf{R}$ for any vector t which is tangent to ∂U at 0. In the local coordinates specified above we are fixing $\xi' = \tilde{\xi}' \in \mathbf{R}^{N-1}$ and assuming that the two solutions ξ_N and $\tilde{\xi}_N$ of the quadratic equation

$$\sigma(0, (\xi', s)) = z$$

in $s \in \mathbf{C}$ both have positive imaginary parts. We say that L_h satisfies the exit condition at 0 if the set of admissible ξ is non-empty.

Theorem 24. *If $\xi \in \mathbf{C}^N$ is an admissible covector and $z = \sigma(0, \xi)$ then under the above conditions there exist $g_h \in C^\infty(U)$ satisfying the boundary conditions* (54) *and also*

$$\operatorname{supp}(g_h) \subseteq \left\{x \in U : |x| < c' h^{1/2}\right\}, \tag{55}$$

$$\lim_{h\to 0} \|g_h\|_2 = c > 0, \tag{56}$$

$$\|L_h g_h - z g_h\|_2 = O(h^{1/2}) \tag{57}$$

as $h \to 0$.

Proof. We put

$$g_h(x) = \alpha(x') f_h(x) + \tilde{\alpha}(x') \tilde{f}_h(x),$$

where

$$f_h(x) = h^{-\gamma} \mathrm{e}^{i h^{-1} \xi \cdot x} \phi(h^{-1/2} x),$$

$$\tilde{f}_h(x) = h^{-\gamma} \mathrm{e}^{i h^{-1} \tilde{\xi} \cdot x} \phi(h^{-1/2} x).$$

In this equation $\gamma = (N+1)/4$ and ϕ is as in the proof of Theorem 23. Also $\xi = (\xi', \xi_N)$ and $\tilde{\xi} = (\xi', \tilde{\xi}_N)$. The coefficients α, $\tilde{\alpha}$ are to be determined. Before continuing, we mention that in the case of Dirichlet boundary conditions we put $g_h = f_h - \tilde{f}_h$, that is $\alpha(x') = -\tilde{\alpha}(x') = 1$; most of the calculations below are much simpler in this situation.

It is immediate from the definition that

$$g_h(x', 0) = h^{-\gamma} \left\{\alpha(x') + \tilde{\alpha}(x')\right\} \mathrm{e}^{i h^{-1} \xi' \cdot x'} \phi_1(h^{-1/2} x'),$$

$$h \partial_N g_h(x', 0) = h^{-\gamma} \left\{\alpha(x') \xi_N + \tilde{\alpha}(x') \tilde{\xi}_N\right\} \mathrm{e}^{i h^{-1} \xi' \cdot x'} \phi_1(h^{-1/2} x').$$

It follows that g_h satisfies the boundary conditions provided

$$i u(x') \left\{\alpha(x') \xi_N + \tilde{\alpha}(x') \tilde{\xi}_N\right\} + w(x') \{\alpha(x') + \tilde{\alpha}(x')\} = 0.$$

This is solved by putting

$$
\begin{aligned}
\alpha(x') &= w(x') + iu(x')\tilde{\xi}_N, \\
\tilde{\alpha}(x') &= -w(x') - iu(x')\xi_N.
\end{aligned}
$$

Since $\xi_N \neq \tilde{\xi}_N$, both α and $\tilde{\alpha}$ cannot vanish near $0'$.

The validity of (55) is immediate. To prove (56) we note that

$$
\begin{aligned}
\|g_h\|_2^2 &= h^{-2\gamma} \int_{\mathbf{R}^N} \left| \alpha(x') \mathrm{e}^{ih^{-1}\xi\cdot x} \phi(h^{-1/2}x) + \tilde{\alpha}(x') \mathrm{e}^{ih^{-1}\tilde{\xi}\cdot x} \phi(h^{-1/2}x) \right|^2 v(x)\, \mathrm{d}^N x \\
&\sim h^{-2\gamma} \int_{\mathbf{R}^N} \left| \alpha(0') \mathrm{e}^{ih^{-1}\xi\cdot x} \phi(h^{-1/2}x) + \tilde{\alpha}(0') \mathrm{e}^{ih^{-1}\tilde{\xi}\cdot x} \phi(h^{-1/2}x) \right|^2 v(0)\, \mathrm{d}^N x \\
&= h^{-2\gamma} v(0) \int_{\mathbf{R}^{N-1}} \phi_1(h^{-1/2}x')^2\, \mathrm{d}^{N-1}x' \\
&\quad \times \int_0^\infty \left| \alpha(0') \mathrm{e}^{ih^{-1}\xi_N x^N} + \tilde{\alpha}(0') \mathrm{e}^{ih^{-1}\tilde{\xi}_N x^N} \right|^2 \phi_2(h^{-1/2}x^N)^2\, \mathrm{d}x^N \\
&= v(0) \int_{\mathbf{R}^{N-1}} \phi_1(s')^2\, \mathrm{d}^{N-1}s' \\
&\quad \times \int_0^\infty \left| \alpha(0') \mathrm{e}^{i\xi_N s^N} + \tilde{\alpha}(0') \mathrm{e}^{i\tilde{\xi}_N s^N} \right|^2 \phi_2(h^{1/2}s^N)^2\, \mathrm{d}s^N \\
&\to v(0) \int_{\mathbf{R}^{N-1}} \phi_1(s')^2\, \mathrm{d}^{N-1}s' \int_0^\infty \left| \alpha(0') \mathrm{e}^{i\xi_N s^N} + \tilde{\alpha}(0') \mathrm{e}^{i\tilde{\xi}_N s^N} \right|^2 \mathrm{d}s^N \\
&> 0
\end{aligned}
$$

as $h \to 0$.

The proof of (57) depends upon writing

$$
L_h g_h - z g_h = k_1 + k_2 + k_3 + k_4,
$$

where

$$
\begin{aligned}
k_1(x) &= \alpha(0')\{L_h f_h(x) - z f_h(x)\}, \\
k_2(x) &= \tilde{\alpha}(0')\{L_h \tilde{f}_h(x) - z \tilde{f}_h(x)\}, \\
k_3(x) &= L_h[\{\alpha(x') - \alpha(0')\} f_h(x)], \\
k_4(x) &= L_h[\{\tilde{\alpha}(x') - \tilde{\alpha}(0')\} \tilde{f}_h(x)]
\end{aligned}
$$

and then estimating each term as before. $\square$

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